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16. ABSTRACT

The report gives Phase II results of a combined experimental/theoretical study to define the mechanisms and kinetics of the formation of NOx and other combustion pollutants. Two experimental devices were used in Phase II. A special flat-flame burner with a controlled-temperature post-flame zone was used to investigate combustion modification techniques used to control NOx emissions: staged combustion, water addition, exhaust gas recirculation, and degree of air preheat. Augmenting the Phase I (unmodified) combustion testing, a novel flow reactor--the adiabatic stirred combustor (ASC)--was built for use in Phase II. The ASC had two distinct zones: a stirred reactor zone, followed by a plug flow zone. Each zone incorporated special provisions to eliminate heat loss from the combustion process. This new device allowed kinetic studies unhindered by mixing or heat transfer limitations. ASC test results were compared with detailed kinetics calculations using a prescreened set of reactions from an evaluation of all possible uni- and bi-molecular reactions for species of importance to methane/air combustion. In contrast to previous comparisons, good matches were obtained for the methane/air system over the entire stoichiometry range. The comparisons showed strong interaction between hydrocarbon species and molecular nitrogen near stoichiometric and fuel-rich conditions.

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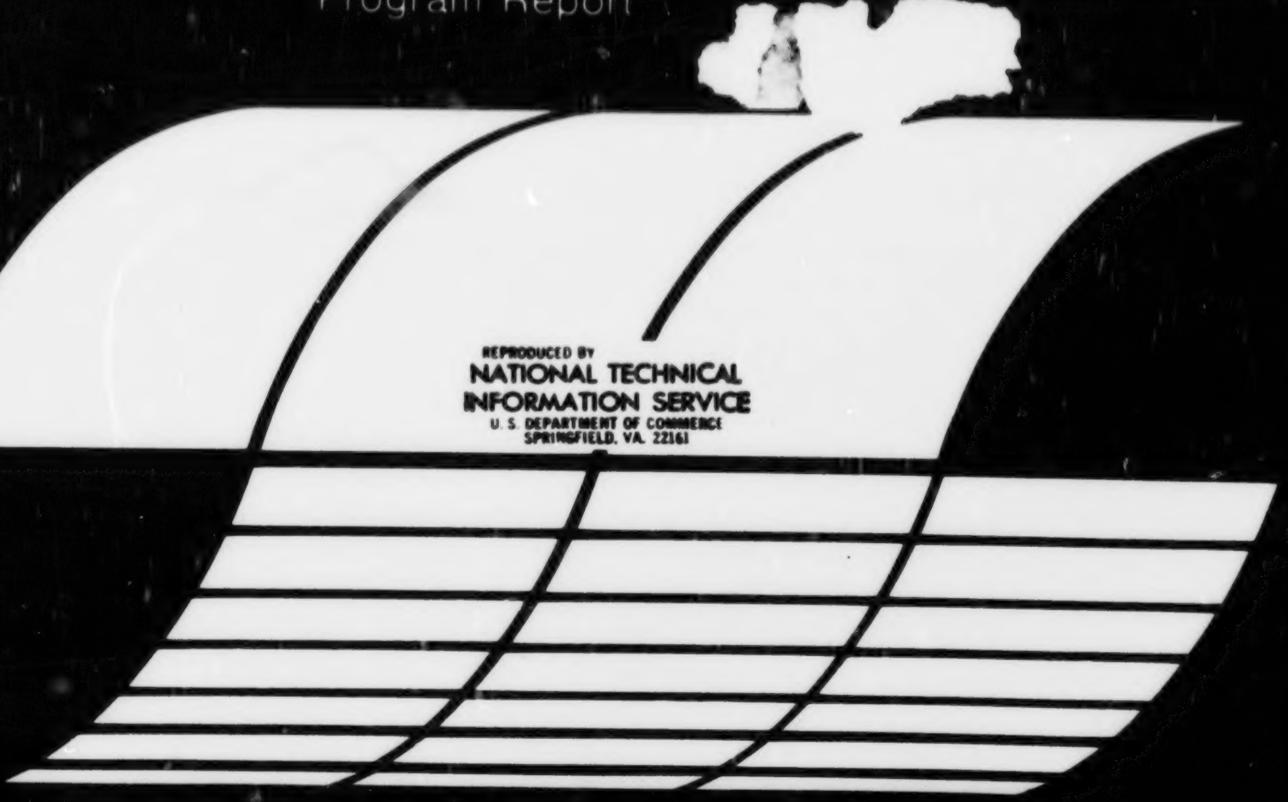
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MECHANISM AND KINETICS OF THE FORMATION OF NO_x AND OTHER COMBUSTION POLLUTANTS

PHASE II. MODIFIED COMBUSTION

by

V.S. Engleman, V.J. Siminski, and W. Bartok

Exxon Research and Engineering Company
P.O. Box 8
Linden, New Jersey 07036

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EPA Project Officer: W. Steven Lanier

Industrial Environmental Research Laboratory
Office of Energy, Minerals, and Industry
Research Triangle Park, NC 27711

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FOREWORD

This report summarizes the results of Phase II of a study on the "Definition of the Mechanism and Kinetics of the Formation of NO_x and Other Pollutants under Normal and Combustion Modification Conditions". This study was conducted by Exxon Research and Engineering Company under Contract 68-02-0224 funded by the Environmental Protection Agency.

The helpful comments and suggestions of Mr. W. S. Lanier, the EPA Project Officer for this contract, are gratefully acknowledged. The skillful assistance of Mr. J. H. Ballentine was invaluable in conducting the laboratory portion of this investigation. The consultation of Professor H. C. Hottel was instrumental in the design of the Adiabatic Stirred Combustor.

SUMMARY

This report describes a study to relate the kinetics and mechanisms of pollutant formation reactions and those of hydrocarbon reactions. An understanding of the chemistry of combustion systems along with the fluid mechanics and heat transfer of specific configurations can lead to an understanding of the details of pollutant formation and control.

Studies of modified combustion techniques used for NO_x emission control were studied with a flat flame burner with a controlled-temperature post-flame zone. Normal combustion was studied with an adiabatic stirred combustor in which fluid mechanical and heat transfer effects were minimized. Preheat temperature and residence time were also varied in the stirred combustor studies. Detailed probing was conducted for stable combustion species.

The Adiabatic Stirred Combustor (ASC) is a new device, designed to take advantage of the capability of the Multiburner (a zirconia muffle furnace capable of achieving temperatures up to 2500 K) to operate without heat loss from the combustion zone and the capability of a stirred reactor to operate under chemically-controlled combustion conditions. Comparison of the ASC data with other stirred reactor data and measurement of the species profiles downstream of the exit plane of the stirred reactor verified that the ASC was operating in a manner comparable to a conventional jet-stirred combustor under comparable conditions and that radial profiles were uniform.

Kinetics calculations were compared with experimental data from the ASC to investigate the mechanism of combustion and NO_x formation under chemically-controlled conditions (i.e. not controlled by mixing or heat transfer limitations). It was found that the calculations for carbon monoxide and hydrogen combustion gave good matches to the experimental results obtained with the ASC, as had been found previously with a nonadiabatic system. In contrast to previous comparisons, where NO_x formation for hydrocarbon/air combustion in a jet-stirred combustor could not be adequately modeled, good matches were obtained for methane/air combustion when a more complete kinetic mechanism was used. The calculations for methane/air combustion indicated strong interaction between hydrocarbon species and molecular nitrogen under certain conditions. The reaction

$$CH + N_2 \rightarrow HCN + N$$

was found to dominate N atom formation under fuel rich conditions and to be a major factor under conditions near stoichiometric air supply. Under fuel lean conditions, the reaction

$$N_2 + O \rightarrow NO + N$$

was found to dominate the production of N atoms. The primary paths from N atoms to NO are

$$N + OH \rightarrow NO + H$$

$$N + O_2 \rightarrow NO + O$$

Further study of the $CH + N_2$ reaction as well as reactions involved in the formation of CH and its precursors is warranted.

1. INTRODUCTION

Under Contract No. 68-02-0224, sponsored by the Environmental Protection Agency (EPA), Exxon Research and Engineering Company (Exxon), has performed a study to relate the kinetics and mechanisms of pollutant formation reactions and those of hydrocarbon reactions. The emphasis in this program to date has been placed on NO_x formation and destruction reactions, as they relate to hydrocarbon combustion.

The experimental tools used previously in these studies have been the Multiburner unit, which can be operated with controlled rates of heat loss and heat addition, and the Jet-Stirred Combustor, in which transport effects are minimized and thus, chemical kinetics govern the rates of combustion and NO_x formation reactions.

In Phase I of this study, a detailed experimental investigation was made with methane and propane fuels, using the Multiburner with premixed, laminar diffusion, and turbulent diffusion flames, varying the mixture ratio and heat removal rates. The flame probing data generated were compared with kinetic analysis, based on parametric studies of the kinetics evaluation.

During the course of this study, a critical review of the literature on the kinetics of pollutant formation and related hydrocarbon reactions was made for the methane/air system (1-1). Recommendations were made on the best available rate information for each reaction.

In Phase II of this study the major objective was to investigate the chemistry of pollutant formation in a chemically controlled system under normal and modified combustion conditions. For this purpose, the Adiabatic Stirred Combustor (ASC) was developed and put into use. The ASC was designed to have two distinct zones: a stirred reactor zone, followed by a plug flow zone. The results from the ASC experiments were compared with detailed kinetics calculations using a pre-screened set of reactions (see Section 3.1.3) from an evaluation of all the possible unimolecular and bimolecular reactions for species judged to be of potential importance in methane/air combustion. Primary attention was focused on understanding reaction paths elucidated by this approach to the calculations. The match of the experimental data to the calculations was used as a guideline to determine gross inconsistencies in the mechanism. Rate-fitting was not done merely to obtain "best-fit" curves but to assess the sensitivity of the results to variations in kinetic parameters. Critical reactions were singled out for further attention in independent studies.

1-1 Engleman, V. S., Survey and Evaluation of Kinetic Data on Reactions in Methane/Air Combustion, Final Report, EPA Contract 68-02-0224, Report No. EPA 600/2-76-003 (January 1976).

2. EXPERIMENTAL

To help elucidate the mechanism of pollutant formation under normal and modified combustion conditions, premixed flat flames and adiabatic stirred combustor flames were studied in the Multiburner with hot and cold walls. This section describes the experimental procedures used in this study and presents the experimental results.

2.1 The Multiburner Furnace

The Multiburner (so-called because it was designed to burn gaseous, liquid or solid fuels at atmospheric pressure) is an electrically heated zirconia tube furnace capable of operating under controlled heat loss conditions. Furnace wall temperatures of 2500°K can be obtained. The idealized primary combustion zone in this study was of a pre-mixed flat-flame type or a well-stirred zone followed by plug flow. In both types of combustion, the post flame reactions are affected by the temperature of the post-flame zones. Since the muffle tube temperature can be varied independently of the flame conditions, a wide range of heat loss rates can be achieved, varying from adiabatic operation to the high loss rates found in water-wall operation. Operation under adiabatic conditions allows study of the flame zone and post-flame zone without the additional complication of heat transfer effects.

The furnace is shown schematically in Figure 2-1. A photograph of the furnace is presented in Figure 2-2. The furnace heating zone has tungsten mesh heating elements and molybdenum radiation shields and is purged with "gettered" argon to extend furnace component lifetimes. High temperature gasketing for the furnace is composed of zirconia felt. Temperatures inside the furnace are monitored with unshielded tungsten-rhenium thermocouples which also serve as the input to a proportional temperature controller for the furnace when operating in the automatic mode. Wall temperatures can also be monitored by optical pyrometry through three sight ports provided in the side of the furnace. The power supply is a 25 KVA AC unit which is also equipped with a thermal watt converter for input to the controller in cases where it is desirable to control power input rather than strictly the temperature of the furnace. The controller on the power supply is also capable of operating in a "manual" mode in which case current input to the furnace is controlled.

The muffle tube in the furnace has a heated length of 38 cm. and the "constant temperature section" of the heated zone is uniform within ±10°K under combustion operation conditions. The muffle tube is quite stable at high temperatures and can be exposed to varying thermal environments in the temperature range above 1600°K. However, extreme care must be exercised in heating up and cooling down the furnace since the zirconia is most sensitive to thermal shock in the temperature range around 1200°K.

FIGURE 2-1

MULTIBURNER FURNACE

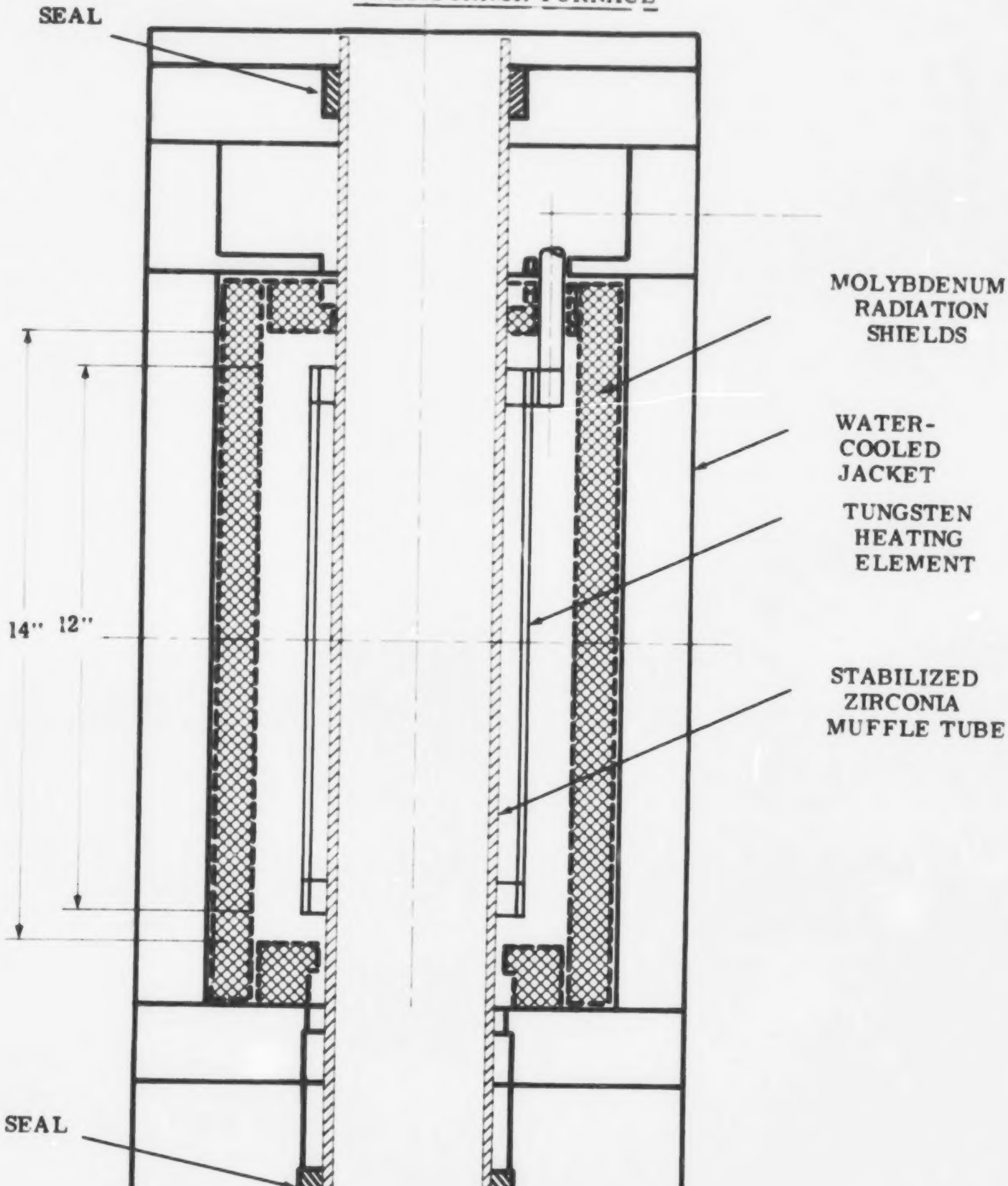
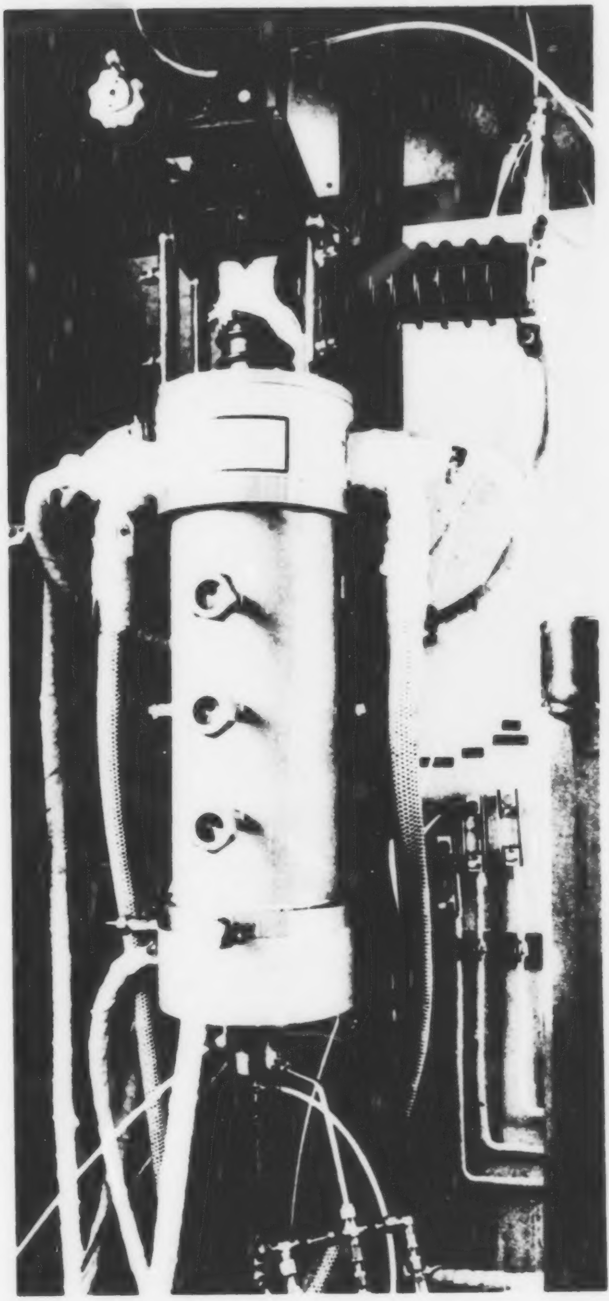

SEAL
MOLYBDENUM RADIATION SHIELDS
WATER-COOLED JACKET
TUNGSTEN HEATING ELEMENT
STABILIZED ZIRCONIA MUFFLE TUBE
14"
12"
SEAL
2-1/2"

Figure 2-2

Multiburner Furnace



The multiburner can operate with the combustion zone wall temperature at any desired level and at the extremes it can either be used to add heat to the combustion zone or, if desired, to remove heat. Thus, the multiburner can operate with all of the flexibility of a laboratory combustor without the high heat loss generally found in small scale devices. This permits the use of the multiburner under combustion conditions that would not be possible with the typical small scale combustor.

2.2 Sampling and Gas Analysis

Combustion gas samples were extracted from the reactor at various radial and axial locations within the primary combustion zone as well as the post flame zone. A water-cooled quartz probe, mounted on a two-degree of-freedom, vernier-operated actuator was utilized to obtain the samples. The interconnecting gas sampling lines were of Teflon which were heated to 150°C to prevent water condensation. Particulate filters and water-cooled condensers were employed at the inlet to the instrument train. Quartz and Teflon materials of construction were used throughout the sampling system to prevent catalytic reduction of NO by CO (2-1).

The exact position of the quartz probe within the reactor was determined from vernier dial and linear distance indicator readings that were located on the two-degree of freedom probe actuator.

The combustion gases were analyzed for NO and NO_x with a Thermoelectron Model 10A Chemiluminescence analyzer. The analysis for NO was accomplished directly while the analysis for NO_x was accomplished by converting the NO_2 (and under certain conditions other nitrogenous compounds) in the stainless steel converter supplied with the instrument to NO and then analyzing for NO.

Analyses for CO and CO_2 were performed with MSA 303 Analyzers of the NDIR type. Stacked cells each with a dual range switch allowed full-scale ranges from 0.1% to 15% for CO and from 0.5% to 25% for CO_2.

Oxygen analysis was performed with a Beckman Model 742 polarographic oxygen analyzer with full scale ranges from 1% to 25%.

Hydrocarbon analyses were performed with a Beckman Model 400 flame ionization analyser with full scale ranges calibrated from 50 ppm to 5% hydrocarbon (as methane equivalent).

2.3 Data Reduction

Experimental data were coded onto computer input forms as taken and were reduced to measured species concentrations by a data reduction program. The data produced in this phase of the program are presented in Appendix A. The data were tabulated according to the type of combustion modification studied.

2-1 Halstead, C. J. and Munro, A. J., Proceedings of the Conference on National Gas Research and Technology, Chicago, 1971.

2.4 Flat Flame Premixed Burner Design

The water-cooled premixed flat flame burner used in this study consisted of a fuel-air mixing chamber and a porous sintered stainless steel grid upon which the flat flame was stabilized. The porous grid provides a uniform velocity profile for the combustion gases entering the furnace tube. A schematic diagram of the flat flame burner is given in Figure 2-3.

2.5 Combustion Modifications in the Flat Flame Burner System

Table 2-1 summarizes the various combustion modifications that were tested in the flat flame burner system with heated and cool furnace walls. Combustion modifications tested were staged combustion, pre-heated air, exhaust gas recirculation, and water addition. The run numbers identify the computer printout sheets which appear in Appendix A.

2.6 Staged Combustion

Figure 2-4 shows a schematic of the experimental setup for studies of staged combustion. The primary air flow rate was controlled with a needle valve and precision rotameter. CH_4 was metered into the flat flame burner through a sonic orifice located immediately upstream of the mixing chamber in order to prevent small pressure fluctuations in the air line from affecting the fuel flow rate. A precision rotameter and needle valve were utilized to control the secondary air flow. The secondary air was injected radially from fifty 0.08 cm. diameter holes into the plug flow zone at an axial location 37.5 cm. downstream of the burner surface. The secondary air flow rate was varied from zero to 50 percent of the total (primary and secondary) air flow rate. Heated and cold wall conditions were tested in this configuration. In the heated wall tests, the wall temperature was varied from 1780 to 2094 K. The secondary injection velocity was calculated to be 5.18 meters/sec. for 25% secondary air injection and 7.92 meters/sec. for 50% secondary air injection when the primary air flow rate was held constant at 15.84 ℓ/min. The gas velocity in the plug-flow zone at the point where the secondary air was injected was about 3.35 meters/sec. at 1773 K.

Gas sample data were obtained at fixed axial locations of 36.75 cm. (before secondary injection) and 85.75 cm. (after secondary injection) from the surface of the flat flame burner. All the cold wall tests (runs 333 through 336) were performed with the gas sample probe located in the exhaust stack of the multiburner 85.75 cm. downstream from the burner. For cold wall conditions, primary zone stoichiometry was varied from 89 to 120% stoichiometric air. Peak NO_x concentrations were found to occur for primary zone stoichiometries close to 100% independent of the secondary air percentage. In the cold-wall tests, the main effect of secondary injection appeared to be simply dilution since the combustion gases had cooled significantly by the point of secondary injection.

Table 2-2 summarizes the test conditions used during the staged combustion runs with hot walls. Primary zone mixture ratios of 50, 60 and 80% stoichiometric air were studied. The overall mixture ratios in the secondary zone were 50, 60, 80, 100 and 120% stoichiometric air.

FIGURE 2-3

FLAT FLAME BURNER

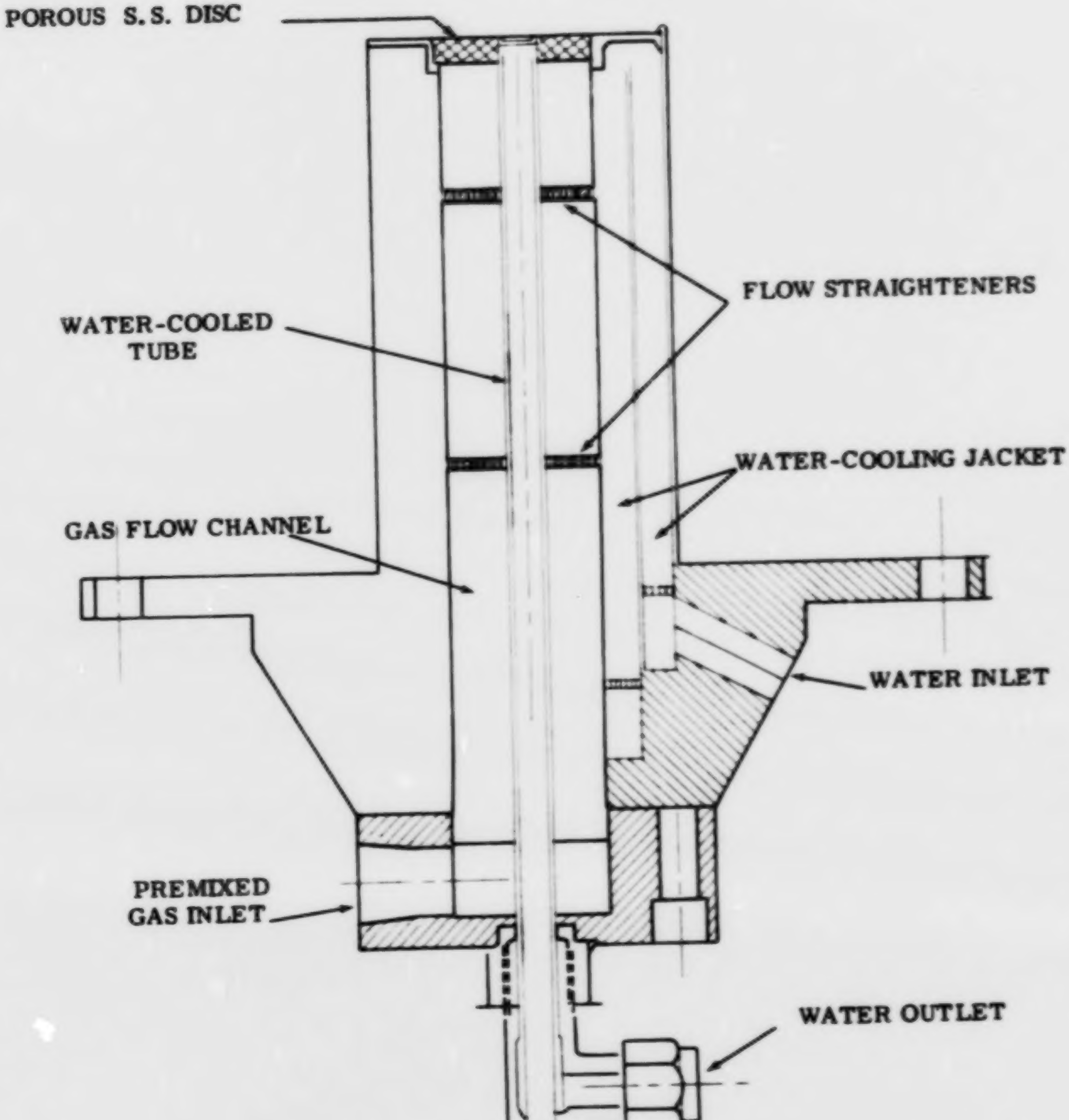

POROUS S.S. DISC
FLOW STRAIGHTENERS
WATER-COOLED TUBE
WATER-COOLING JACKET
GAS FLOW CHANNEL
WATER INLET
PREMIXED GAS INLET
WATER OUTLET
WATER INLET

TABLE 2-1

PREMIXED FLAT FLAME COMBUSTOR RUN IDENTIFICATION FOR CHEMICAL SPECIES CONCENTRATION PROFILES

CH_4 / Air Mixtures

Staged Combustion

Run #	Firing Rate ℓ/min.	% Secondary Air	Wall Temperature K
333	18.5	0-25	Cold[(a)]
334	18.5	30-34	Cold
335	18.5	0-25	Cold
336	18.5	30-34	Cold
365	15.9	0-50	1780
369	15.9	0-50	1780
370	15.9	0-34	2094

Pre-Heated Air

		Pre-Heat Temperature (°K)	
364	15.9	298	1857
367	15.9	298	2042
368	15.9	298	1857
371	15.9	443	1985
372	15.9	443	2156
377	15.9	313-353	2224

Exhaust Gas Recirculation

		Recirculation Ratio $\left(\frac{\text{volume recirculated}}{\text{initial volume}}\right)$	
374	15.9	0-0.50	1831
375	15.9	0-0.25	2027
376	15.9	0-0.10	2163

Water Addition to Reactants

		Percent H_2O (volume)	
378	15.9	0-2.0	2073

(a) No external heat applied to the combustor walls.

FIGURE 2-4

SCHEMATIC OF FLAT FLAME BURNER SYSTEM FOR STUDIES OF UNMODIFIED AND STAGED COMBUSTION

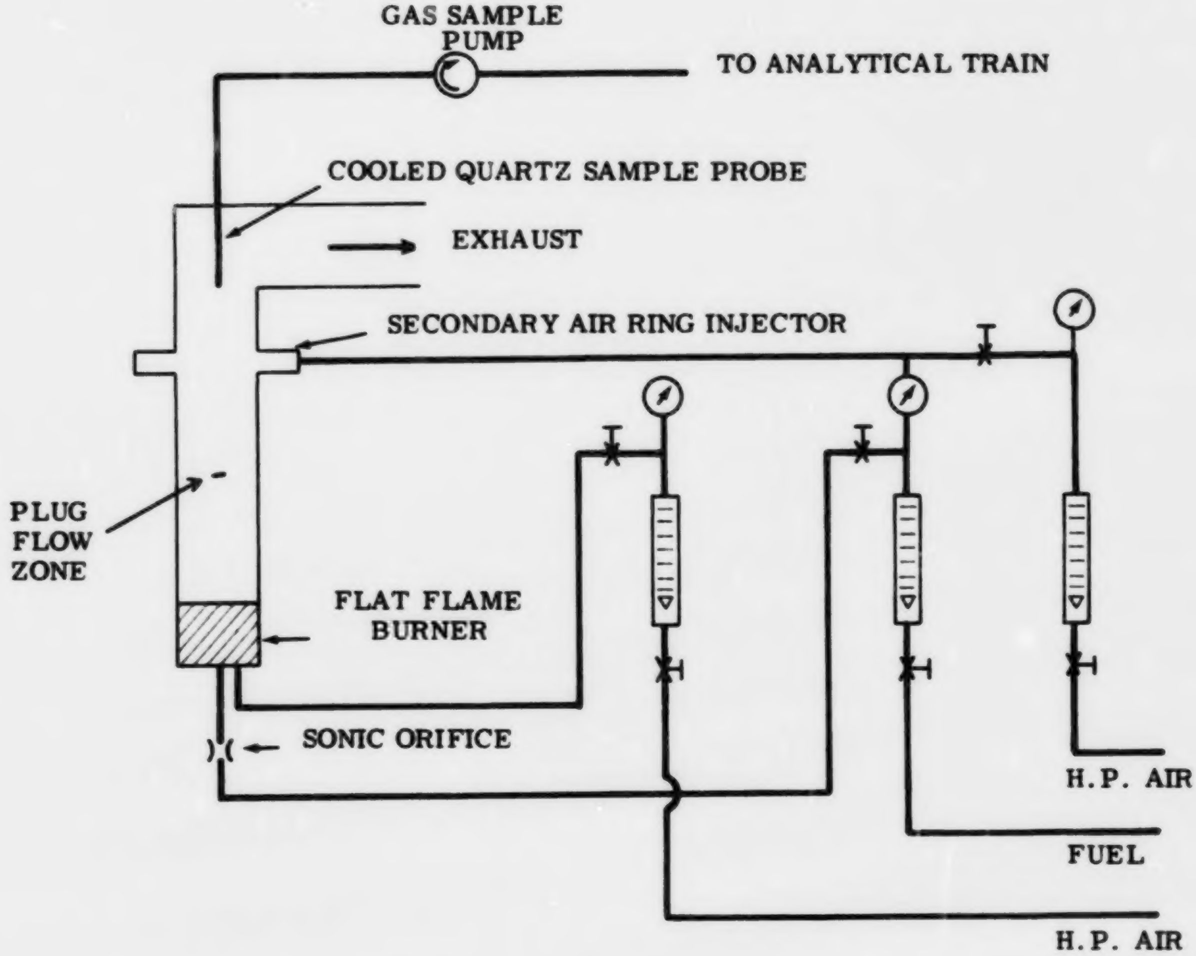

GAS SAMPLE PUMP
TO ANALYTICAL TRAIN
COOLED QUARTZ SAMPLE PROBE
EXHAUST
SECONDARY AIR RING INJECTOR
PLUG FLOW ZONE
FLAT FLAME BURNER
SONIC ORIFICE
H.P. AIR
FUEL
H.P. AIR

TABLE 2-2

CENTERLINE NO_x CONCENTRATIONS IN PREMIXED FLAT-FLAME BURNER WITH CH_4/AIR AND STAGED COMBUSTION

Run #	Primary Pct. Stoich. Air	Primary* NO (ppm)	Overall Pct. Stoich. Air	Overall** NO_x (ppm)	Wall K
365	50.8	0	50.8	0***	1780
			79.7	0***	1780
			100.1	8	1780
369	60.1	3	60.1	2***	1780
			100.1	9	1780
			120.0	7	1780
370	79.2	42	79.2	38***	2094
			101.7	28	2094
			119.6	25	2094

* Axial distance 37.3 cm

** Axial distance 87.1 cm

*** Under fuel rich conditions, the number shown represents the concentration of NO. Measurements were taken far downstream of the flame zone and the NO_2 concentrations represented only about 5% of the total NO_x in most cases.

When the primary zone was maintained at 50% stoichiometric air, no NO was found in the primary zone, and only when the overall stoichiometry reached 100% was 8 ppm of NO_x measured. With the primary zone at 60% stoichiometric air, a small amount of NO (3 ppm) was measured in the primary zone. However, even with secondary air injection, the increase in NO_x was not very large; NO_x concentration reached 9 ppm when the overall stoichiometry was 100% but dropped off to 7 ppm at an overall stoichiometry of 120%. When the primary zone was maintained at 80% stoichiometric air 42 ppm of NO was formed in the primary zone. As secondary air was added, the NO_x concentration decreased by approximately the amount that would be caused by dilution, indicating no significant increase in NO_x caused by secondary combustion.

Run No. 365, with the primary zone at 50% stoichiometric air, illustrates the effect of secondary air injection on the plug flow zone combustion species. The data show that with no secondary injection, the unburned hydrocarbon concentration measured at an axial distance of 85.75 cm. was 2900 ppm. With secondary injection to bring the overall stoichiometry to 80% and 100% the hydrocarbons decreased to 530 ppm and 7 ppm, respectively. The large change in hydrocarbons caused by secondary injection cannot be accounted for by dilution. The low hydrocarbon and CO concentrations resulting from secondary injection indicate that efficient combustion was achieved.

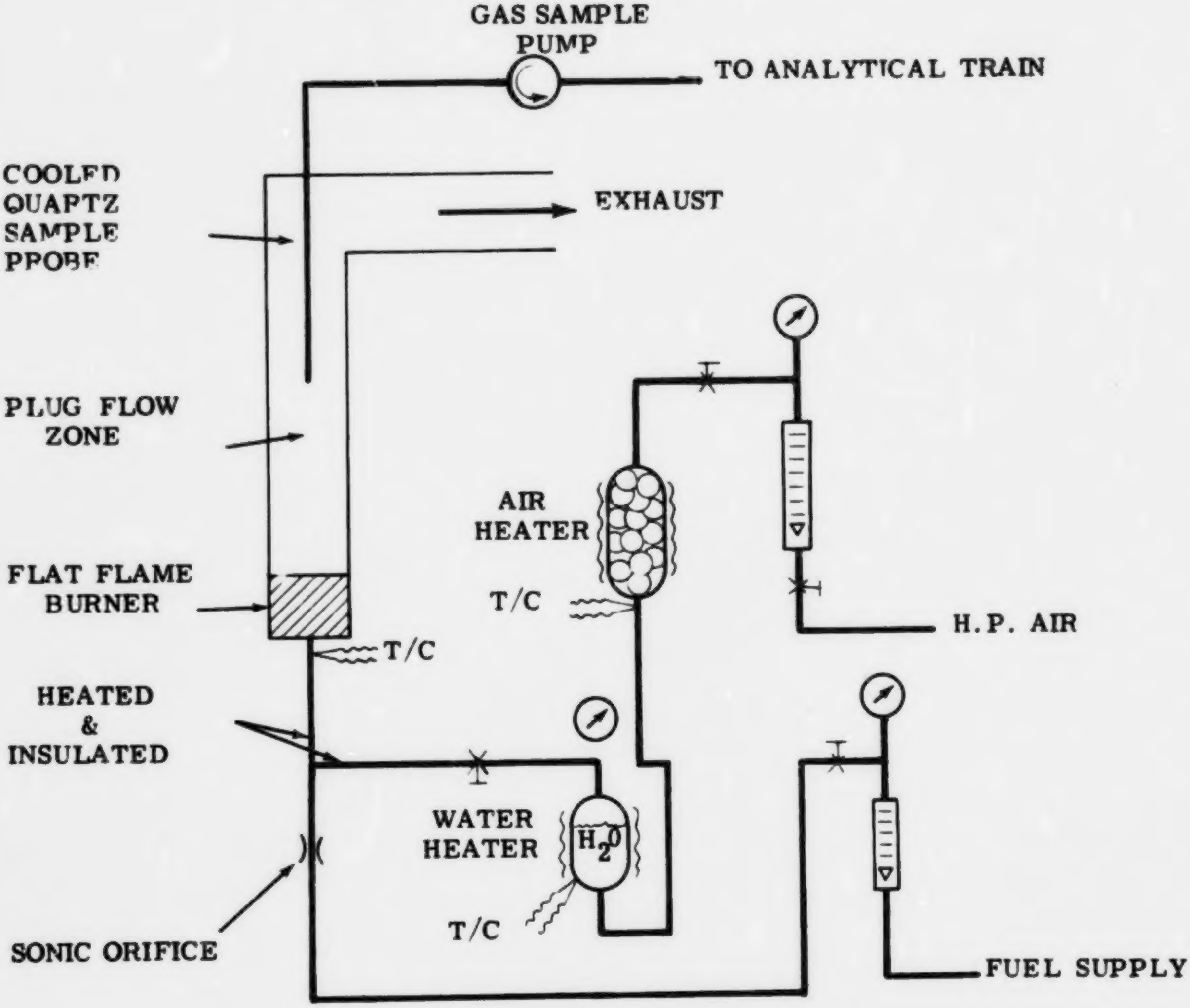
2.7 Preheated Air and Water Addition

Figure 2-5 is a schematic diagram showing the experimental arrangement of the multiburner furnace with the flat flame burner for experiments conducted with preheated air and water addition studies. The combustion air was preheated *via* an electrically heated stainless steel vessel which contained ceramic spheres for increased heat transfer. The temperature of the air was thermostatically controlled by a thermocouple inserted into the vessel. Bypass valves were available in order that the air heater could be eliminated from the air system when desired. As in the unmodified combustion tests with the flat flame burner, the fuel (CH_4) and preheated air were mixed inside the burner body just prior to their flow through the porous disc. A thermocouple located in the mixing section provided temperature data.

Water addition to the reactants was accomplished by bubbling the air through a pressurized, heated stainless steel vessel containing water. The maximum amount of water added was 2% by volume of the total air plus fuel flow (about 20% of the fuel by volume). The water concentration was calculated from the vapor pressure of water at the known temperature and pressure of the water vessel. Bypass valves were provided for tests that were performed with no water addition.

FIGURE 2-5

SCHEMATIC OF FLAT FLAME BURNER FOR PREHEATED AIR AND WATER ADDITION STUDIES


GAS SAMPLE PUMP
TO ANALYTICAL TRAIN
COOLED QUARTZ SAMPLE PROBE
EXHAUST
PLUG FLOW ZONE
AIR HEATER
T/C
H.P. AIR
FLAT FLAME BURNER
T/C
HEATED & INSULATED
WATER HEATER
H_2O
T/C
SONIC ORIFICE
FUEL SUPPLY

The experimental conditions for air preheat and water addition are shown in Table 2-1 and the data are given in Appendix A. Two levels of preheat were selected, 298°K (representing no preheat) and 443°K. An additional run was performed in which the preheat temperature was varied between 313°K and 353°K. The firing rate was maintained at 15.87 l/min. and the walls were maintained at the adiabatic flame temperature. Wall temperature differences are illustrated by the following:

119% stoichiometric air
25°C air - 2042°K wall
170°C air - 2156°K wall
120°C air - 2073°K wall (with 2% water)

140% stoichiometric air
25°C air - 1857°K wall
170°C air - 1985°K wall

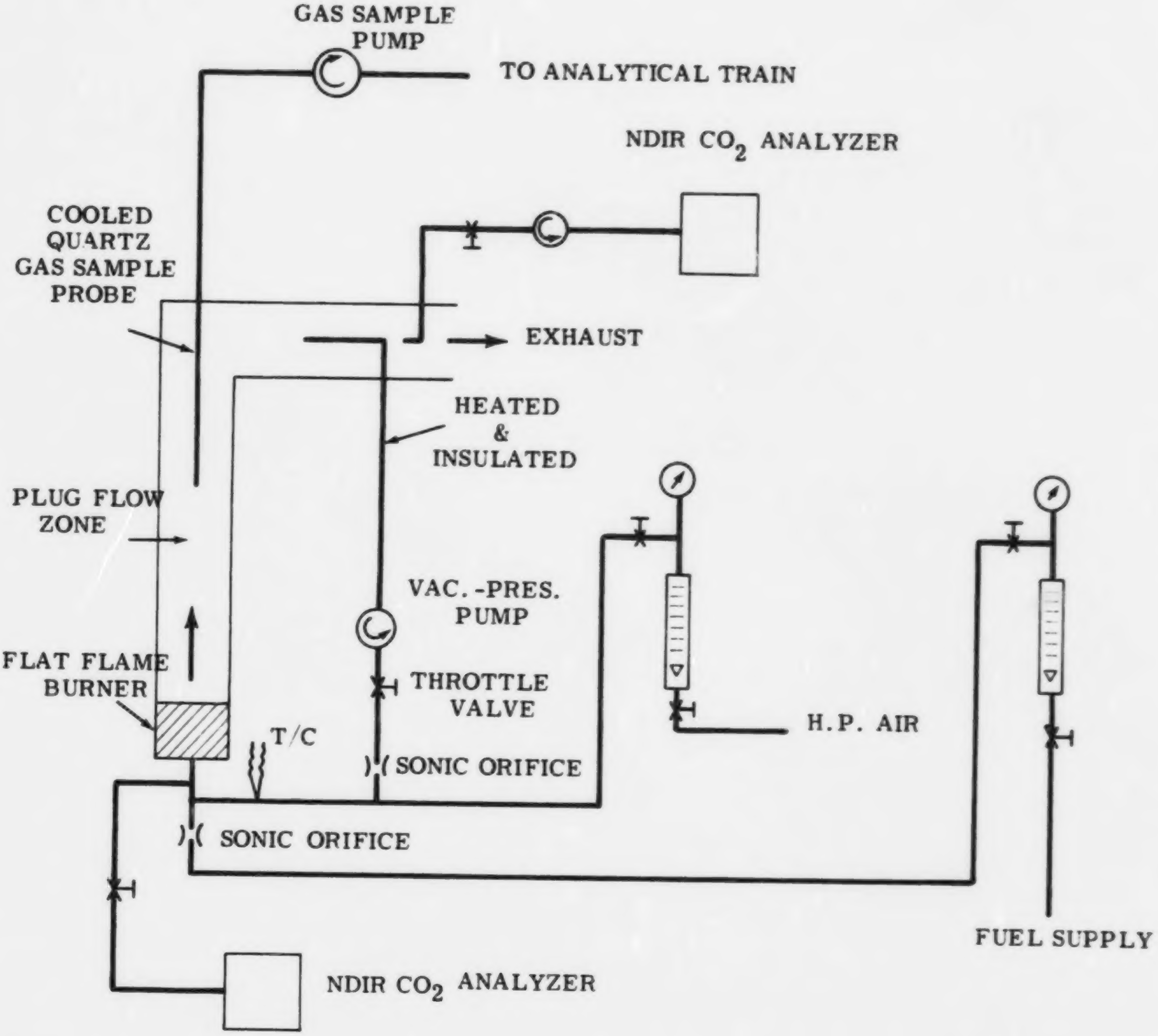
At 119% stoichiometric air, at a distance of 25 cm. from the burner face, NO_x was 83 ppm with no preheat, 190 ppm with preheat and 53 ppm with water addition. Near the burner face (0.6 cm), however, the NO_x measurements were 22 ppm for no preheat, 16 ppm with preheat and 17 ppm with water addition. The behavior of NO_x near the burner and far downstream in the post-flame zone bears further discussion. Near the burner, NO_x is found to be lower in the preheated case, while further downstream it is higher in the preheated case. The Zeldovich mechanism is considered to dominate post-flame NO_x formation under fuel lean conditions. However these results, which indicate lower NO_x concentrations near the burner face with preheat could provide support for non-Zeldovich NO_x in the flame zone. More rapid burnout of the active intermediates in the preheated case could cause a decrease in flame zone NO_x. Complete interactions between hydrocarbon fragments, nitrogen-containing species and oxygen-containing species are involved and possible mechanisms will be discussed in Section 3. There was an apparent lengthening of the flame zone in the water addition case as evidenced by the presence of hydrocarbons (>1%) at a distance of 0.1 cm from the burner face, while none were measured without water addition. Further investigation of these phenomena from both an experimental and theoretical approach appears to be warranted.

2.8 Exhaust Gas Recycle

A schematic diagram of the exhaust gas recycle system utilized with the flat flame burner/multiburner furnace is presented in Figure 2-6. A high temperature bellows pump having a capacity of 34 l/min. was used to withdraw the combustion gases from the multiburner exhaust stack through a 1.27 cm. diameter probe which was located on the centerline of the stack; facing into the exhaust stream. The pump had a discharge pressure of 210 kPa. The combustion gases were injected into a 1.27 cm. diameter mixing section with the primary combustion air. The entire gas recycle system was electrically heated and thermally insulated in order to maintain the temperature of the gases above the dew point of the mixture. The amount of gas withdrawn through the recycling pump was determined by measuring with NDIR analyzers the CO_2 concentrations in the multiburner exhaust stack and the section where the primary air supply was mixed with the exhaust gases. Since the total air flow rate was known and the concentration of CO_2 at both locations was measured, the amount of gas recycled was determined.

FIGURE 2-6

SCHEMATIC OF FLAT FLAME BURNER FOR EXHAUST GAS RECYCLE STUDIES


GAS SAMPLE PUMP
TO ANALYTICAL TRAIN
NDIR CO_2 ANALYZER
COOLED QUARTZ GAS SAMPLE PROBE
EXHAUST
HEATED & INSULATED
PLUG FLOW ZONE
VAC.-PRES. PUMP
FLAT FLAME BURNER
THROTTLE VALVE
T/C
SONIC ORIFICE
H.P. AIR
SONIC ORIFICE
FUEL SUPPLY
NDIR CO_2 ANALYZER

The conditions for exhaust gas recycle are shown in Table 2-3 and the experimental data are given in Appendix A. An air leak in the sampling system was discovered after the data were taken. While the data in the Appendix are given as taken, the results discussed here are corrected for the leak. Three different exhaust gas recycle rates were evaluated; ten percent (adiabatic temperature of 2163°K), twenty-five percent (2027°K) and fifty percent (1831°K). The firing rate in the primary combustion zone was 15.876 l/min. and the overall mixtures were maintained at 100 percent stoichiometric air. Additional data were taken with no recycle at each temperature condition. (The use of 100% stoichiometric air eliminates the need for corrections in stoichiometry caused by residual oxygen or fuel components in the exhaust gas).

At a distance of 33.3 cm. from the burner face the NO_x concentration was 156 ppm with 10% recycle (2163°K), 60 ppm with 25% recycle (2027°K) and 8 ppm with 50% recycle (1831°K). For comparison with the above results, when no recycle was used by the wall temperature was held constant, the NO_x level was 237 ppm (vs. 125 ppm with 10% recycle) with 2163°K walls, 105 ppm (vs. 60 ppm with 25% recycle) with 2027°K walls and 74 ppm (vs. 8 ppm with 50% recycle) with 1831°K walls. The differences noted in the NO_x levels are slightly greater than would be expected from the combined effects of decreased residence time and increased dilution during flue gas recycle. (The corrections for dilution are shown in Table 2-3. No correction was made for residence time.) There do not appear to be major chemical effects caused by the recycle which are discernible at large distances from the burner face thus the effect appears to be primarily thermal.

2.9 Adiabatic Stirred Combustor

In Phase I of this program, a jet-stirred combustor with heat loss to the surroundings was used. The behavior of this jet-stirred combustor had been shown to approximate that of a well-stirred system for NO_x formation in simple non-hydrocarbon flames under kinetically controlled conditions (2-2). However, because of the extremely strong temperature dependence of many of the elementary reaction rates that play a role in the formation of NO_x in hydrocarbon flames, it was concluded at the end of our Phase I studies that it would be desirable to construct a reactor system that is capable of operation in the absence of thermal gradients in the flame and downstream combustion gases. This would allow comparison of theory and experimental data under even better defined conditions. With the constraint imposed that mass diffusional gradients should be eliminated (or at least minimized) as well, it was decided that an adiabatic stirred reactor was needed that, if successfully developed, could operate in the absence of both thermal and mass diffusional gradients. This section of the present report describes the features of the adiabatic stirred combustor (ASC) developed. Subsequent sections describe its operation and the verification of the premise that indeed it could be operated without significant mass and thermal gradients.

2-2 Engleman, V. S. and Bartok, W., Phase I Final Report (companion report in this series).

TABLE 2-3

EFFECT OF EXHAUST GAS RECYCLE ON NO_x

(Firing Rate 14.603 l/min.)

Run #	% Recycle	Adiabatic Temp. (°K)	NO_x As Measured (PPM)	NO_x Corrected For EGR Dilution (PPM)
376	0	2163	237	237
376	10	2163	156	173
375	0	2027	105	105
375	25	2027	60	80
374	0	1831	74	74
374	50	1831	8	16

The adiabatic stirred combustor (ASC) was designed to represent a segment of the well-known Longwell/Weiss (2-3) jet-stirred reactor. The output combustion rate achieved in the well-stirred reactor is kinetically limited when the mixing is maintained at the proper level (2-4). The intense mixing of the reactants in the well-stirred reactor is due to its symmetrical geometry and the number and diameter of orifices in the injector which introduces sonic velocity jets of pre-mixed reactants into the combustion zone. The recirculation zones established around each of the sonic jets promotes intense mixing of the reactants with the hot combustion products.

The adiabatic-stirred-combustion section was followed by a plug flow zone that was designed to promote as little recirculation as possible in the area adjacent to the walls of the plug flow zone. Some very slight recirculation was present, however, because of the finite wall thickness (0.157 cm.) of the stirred combustor section.

The ASC consisted of three components; an injection tube, the well-stirred combustion chamber and the plug flow tube. A schematic diagram of the ASC assembly is given in Figure 2-7. All components were made of stabilized zirconia*. The injector tube consisted of a 0.635 cm. outer diameter tube sealed at one end by a hemisphere that contained seven symmetrically spaced 0.0406 cm. diameter holes drilled with diamond tip bits. The holes on the 0.254 cm. diameter hole circle were drilled such that the included angle between opposite holes was 48°. This injector configuration prevented the gas jets from impinging upon the reactor walls. The injector tube had a water-cooled stainless steel "finger" inserted into its 0.447 cm. I.D. such that the tip of the "finger" was within 0.157 cm. of the hemispherical end of the ZrO_2 tube. The annular space between the water cooled "finger" and the I.D. of ZrO_2 tube was 0.081 cm. This small cross sectional area allowed the air-fuel mixture to remain cool and thus prevented any pre-reaction before injection into the stirred combustion chamber. Flash-back was prevented by the high injection velocity (sonic) of the seven jets. A schematic diagram of the ZrO_2 injector is shown in Figure 2-8.

The well-stirred combustion chamber was made of a standard 2.5 cm. outer diameter ZrO2 crucible having 0.157 cm. thick walls. The height of the flat-topped crucible was 2.22 cm. Thirty-seven 0.157 cm. diameter holes were drilled with diamond bits, on an equilateral triangle pattern having 0.343 cm. sides. The outermost holes, in some instances, actually touched the inner wall of the crucible. This design limited the number of "dead-zones" where recirculation could have taken place. A schematic diagram of the well-stirred combustion chamber is shown in Figure 2-9.

2-3 Longwell, J. P. and Weiss, M. A., Ind. Eng. Chem. 47, 1634 (1955).

2-4 Hottel, H. C., Williams, G. C., and Miles, G. A., Eleventh Symposium (International) on Combustion, p. 771, the Combustion Institute, 1967.

* Supplied by ZIRCOA, P. O. Box 9583, Solon, Ohio 44139. Composition #1192.

FIGURE 2-7

CROSS SECTIONAL VIEW OF ASC ASSEMBLY

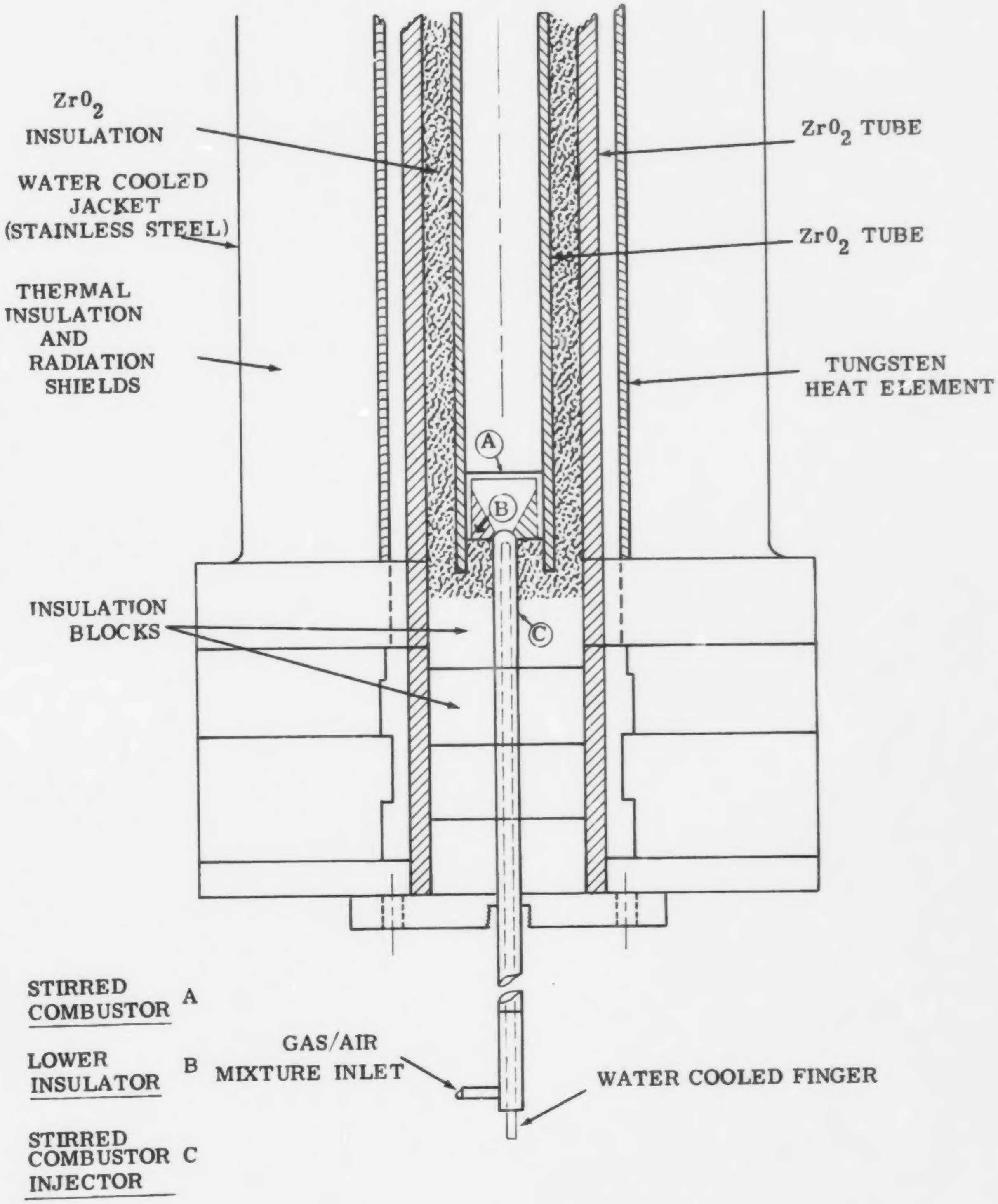

Zr0$_2$ INSULATION
WATER COOLED JACKET (STAINLESS STEEL)
THERMAL INSULATION AND RADIATION SHIELDS
Zr0$_2$ TUBE
Zr0$_2$ TUBE
TUNGSTEN HEAT ELEMENT
A
B
C
INSULATION BLOCKS
STIRRED COMBUSTOR A
LOWER INSULATOR B
STIRRED COMBUSTOR INJECTOR C
GAS/AIR MIXTURE INLET
WATER COOLED FINGER

FIGURE 2-8

ZrO_2 COMBUSTION TUBE INJECTOR

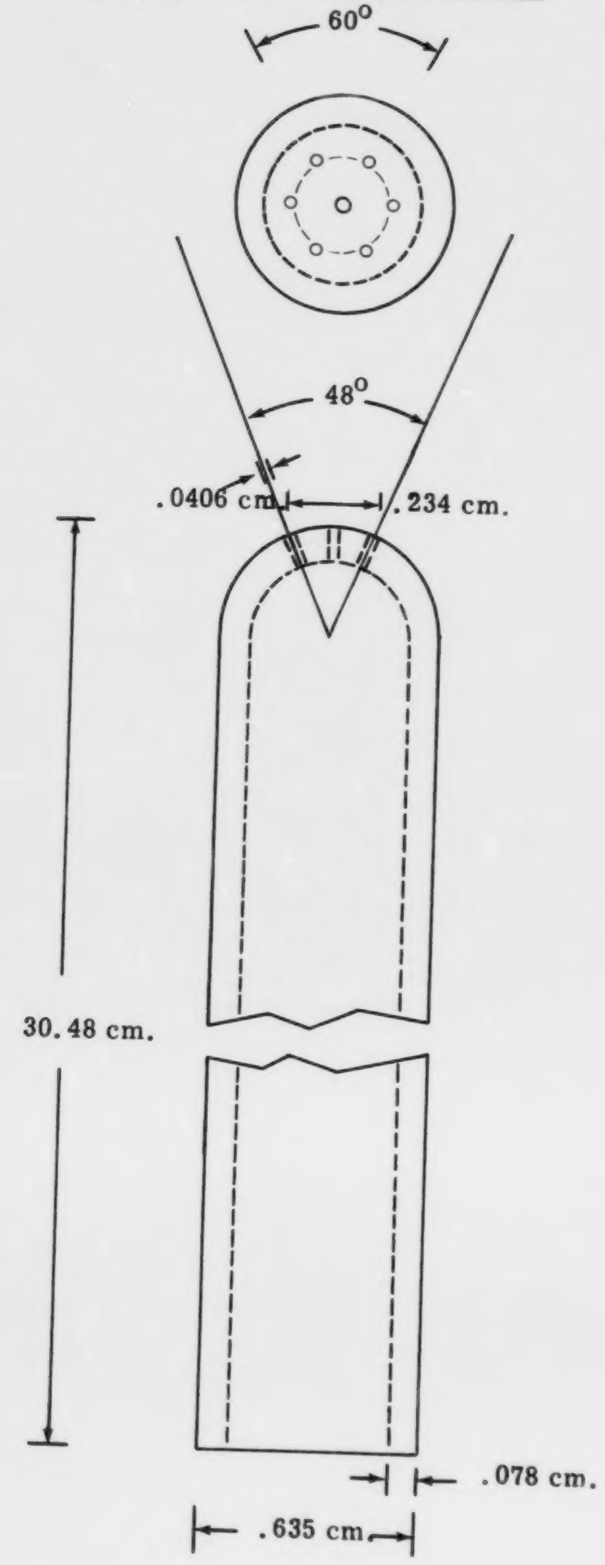
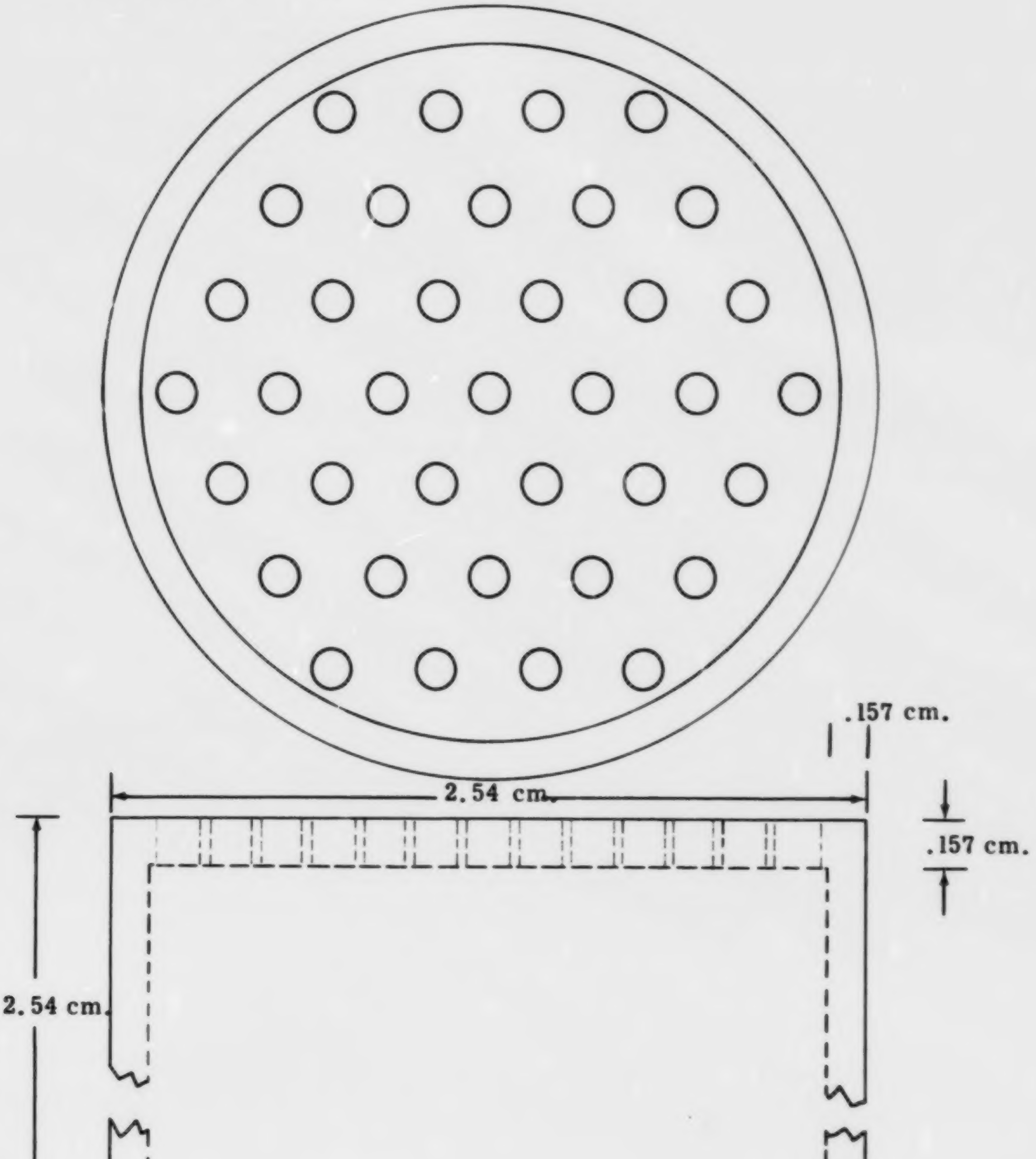

60°
48°
.0406 cm.
.234 cm.
30.48 cm.
.078 cm.
.635 cm.

FIGURE 2-9

ZIRCONIA ASC WELL-STIRRED COMBUSTION CHAMBER INJECTOR DESIGN

SCALE: 5/1

DRILL 37 HOLES:
.157 cm. DIAM. ON .343 cm. CENTERS.


.157 cm.
2.54 cm.
.157 cm.
2.54 cm.

In order to prevent impingement of the fuel-air mixture jets upon the side walls of the combustor, a hollow conical transition piece was molded from ZrO_2 material such that the included angle of the transition was 70°. The 0.635 cm. diameter injector tube was located within the base of the conical transition. The seven injector jets stirred the reaction within the flat topped conical-walled combustion chamber. The conical volume within the crucible, including the volume of the 37, 0.157 cm. diameter holes, was determined to be 4.9 cm^3 by measuring the volume of mercury required to fill the volume with the holes covered up to the point where the 0.635 cm. hemispherical injector tube was located.

The combustion products were exhausted from the 37 holes of the combustion chamber, at subsonic velocities in order to avoid the creation of another well-stirred zone into the 2.5 cm. diameter x 43.18 cm. long plug-flow zone tube. The laminar* flow of combustion species within the plug-flow zone was sampled via the quartz-lined, water cooled stainless steel probe which was manually manipulated with an actuator capable of moving in both axial and radial directions.

Table 2-4 summarizes the typical operating characteristics of each of the three portions which made up the ASC.

2.9.1 Operation of the ASC

The ASC was designed to be installed into the multiburner furnace with a minimum of down-time such that burners of various geometries could easily and rapidly be inserted into the electric furnace. Figure 2-7 shows that the location of the stirred combustor relative to the lower edge of the tungsten heating element was such that the combustor as well as the plug-flow tube were uniformally heated to avoid regions of non-adiabatic conditions. The heavy thermal insulation surrounding the injector tube minimized the heat transfer between the tungsten heating element and the injector tube. Pre-reaction of fuel and air at furnace temperature up to 2300°K was prevented by a water cooled "finger" that was inserted into the injector tube. A 0.157 cm. gap between the inch of the water cooled "finger" and the hemispherical tip of the injector tube minimized heat losses in the ASC that may have been induced by the presence of the cooled "finger". In this fashion, the reactant mixture was always injected at uniform temperatures and velocities higher than the flame propagation velocities for mixtures of air with hydrocarbons, carbon monoxide or hydrogen.

The electric furnace was never allowed to cool below 1200°K after being energized since phase transformation within the ZrO_2 components occurs below this temperature after the parts have been exposed to temperatures in excess of 1400°K.

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* Average flow velocity in the 2.5 cm. diameter tube at 16.98 l/min. flow rate and 2420°K was calculated to be 4.57 meters/sec. The calculated Reynolds number under these conditions was 214. Therefore, the flow was in the laminar region.

The average flow velocity in one, 0.157 cm. diameter hole of the crucible under similar conditions stated above was calculated to be 30.5 meters/sec. The Reynolds number was 34, hence the flow was laminar. In the above calculations the working fluid was assumed to be air which has an absolute viscosity of approximately 0.08 centipoise at 2420°K. (Maxwell, J. B., Data Book on Hydrocarbons, D. Van Nostrand Co., Inc., N. Y. 1950.)

TABLE 2-4

TYPICAL OPERATING CONDITIONS FOR THE ASC STIRRED COMBUSTION ZONE

- Reactor Pressure = 102 kPa.
- ASC Reactor Volume: 4.9 cm^3. (measured)
- Reactant Flow Rates: 17 l/min air, 2.8 l/min Fuel
- Reactor Temperature: 1500° - 2200°K
- Average Reactor Residence Time: 2×10^{-3} sec @ 1800°K
- Average Reynolds Number @ Exit Plane of one .157 cm. hole: 34
- Average Exit Jet Velocity: 28.3 meters/sec calculated from air flow measurement.

PLUG-FLOW ZONE CONDITIONS

- Length of Plug-Flow Zone: 43.18 cm.
- Average Velocity @ 1800°K: 3.96 meters/sec
- Average Residence Time: 0.106 sec
- Reynolds Number: 214

FUEL-AIR INJECTOR

- ΔP across injector 105-140 kPa.
- Injection Velocity: 312 meters/sec

Normal operating procedure consisted of setting the furnace temperature controller at the calculated adiabatic combustion temperature for a given fuel-air mixture with either H_2, CH_4, C_3H_8 or CO as fuels. The furnace temperature was then allowed to equilibrate with the water cooled gas sample probe withdrawn, so as not to cause cooling of the interior furnace walls. The automatic proportional temperature controllers compensated for temperature changes when the probe was inserted into the plug flow tube after the furnace had equilibrated. The gas sample probe was moved in the X and Y directions until sufficient gas analysis data were obtained at a given fuel-air mixture, or by varying one of the test conditions when modified combustion experiments were conducted. Because of the sensitivity of combustion species concentrations to small changes in fuel flow rate all of the test data at various axial and radial probe locations were obtained at fixed fuel settings before any fuel flow rate changes were made. When the fuel flow rate was intentionally altered to obtain a different equivalence ratio (ϕ) the measured combustion species distribution at the new ϕ was compared to a set of base-line data taken at a set of reference coordinates within the post flame zone to assure comparability on different days.

Combustion species concentration profiles were obtained in the axial direction between 0.127 and 25.4 cm. from the surface of the well-stirred combustor and to within 0.033 cm. of the side walls of the plug flow tube. It was not possible to probe any nearer to these surfaces without causing damage to the stabilized zirconia components, due to thermal shock failures caused by allowing the cooled sample probe to contact the hot surfaces.

When combustion modification conditions such as exhaust gas recycle and staged combustion were carried out the gas sampling probe was either removed completely from the plug flow tube or withdrawn to a non-interrupting position.

2.9.2 Normal Combustion

In order to verify that the ASC was producing a uniform gas composition at the surface (axial distance = 0.127 cm.) of the burner, a series of runs were performed with various mixtures of CH_4 or C_3H_8 and air at different firing rates. The results of these tests are summarized in Tables 2-5, 2-6 and 2-7. These data were obtained with the quartz sampling probe located at five different radial points across the 2.54 cm. diameter of the burner head and at six different axial distances. As can be seen from the data, most of the gas sampling was performed in a zone close to the burner. The data from Tables 2-5 and 2-7 are plotted in Figures 2-10 and 2-11. Had inefficient mixing occurred inside the ASC, variations in NO_x concentrations would have been observed in the detailed probing of the gas stream in the zone adjacent to the ASC. The NO_x concentration data indicate that the concentrations were quite uniform across the diameter of the ASC for a fixed axial position. The run identification schedule for the methane and propane normal combustion tests are summarized in Table 2-8. Detailed combustion species data may be found by locating from Table 2-8 the corresponding run number in the Appendix, that contains the computer print-out data sheets.

TABLE 2-5

RADIAL PROFILES OF NO_x CONCENTRATION ADIABATIC STIRRED COMBUSTOR C_3H_8/AIR MIXTURES @ 1873°K

Axial Distance(cm)	NO_x Concentration (PPM)					
	0.127	.635	1.27	1.90	2.54	8.13
Radial Distance(cm)		140 Percent Stoich. Air				
-0.762	7	8	6	6	7	7
-0.381	6	9	6	6	6	10
0.0	6	7	6	6	6	7
0.381	9	9	7	7	7	17
0.762	9	8	6	6	6	16
		100 Percent Stoich. Air				
-0.762	13	15	16	15	16	
-0.381	13	15	16	17	16	
0.0	14	13		14	15	
0.381	14	15		14	16	
0.762	14	16		16	15	
		93 Percent Stoich. Air				
-0.762	20	25	25	28	28	
-0.381	22	24	26	28	28	
0.0	22	21	21	22	22	26
0.381	23	24	23	22	23	
0.762	24	23	24	23	23	
		86 Percent Stoich. Air				
-0.762	29	34	32	34	35	
-0.381	31	31	32	35	34	
0.0	32	31	30	30	31	42
0.381	28	28	28	29	29	
0.762	29	29	27	28	29	
		80 Percent Stoich. Air				
-0.762	29	38	38	34	29	
-0.381	28	30	32	36	31	
0.0	35	28	29	31	32	45
0.381	29	28	29	24	31	
0.762	30	31	28	30	29	
		70 Percent Stoich. Air				
-0.762	34	34	35	34	35	43
-0.381	35	36	35	36	36	44
0.0	36	31	33	34	35	46
0.381	36	35	35	36	36	44
0.762	37	35	35	34	35	45
		64 Percent Stoich. Air				
.762	33	22	26	32	35	
.381	31	18	21	28	32	
0	35	28	32	31	33	46
.381	31	38	32	32	32	
.762	33	29	32	31	33	

TABLE 2-6

RADIAL PROFILES OF NO_x CONCENTRATION ADIABATIC STIRRED COMBUSTOR (ASC) CH_4/AIR MIXTURES @ 1873°K

	NO_x Concentration (PPM)			
Axial Distance (cm)	0.635	1.27	1.90	2.54
Radial Distance (cm)	Percent Stoich. Air: 112			
-0.508	28		32	35
-0.254	27		33	33
0.0	27		33	33
0.254	26		32	34
0.508	27		33	35
	Percent Stoich. Air: 64.2			
-0.508		1	1	1
-0.254		1	1	1
0.0	0	0	1	2
0.254		1	1	1
0.508		1	1	1

TABLE 2-7

EFFECT OF MIXTURE RATIO ON NO_x CONCENTRATION PROFILES CENTERLINE OF THE ADIABATIC STIRRED COMBUSTOR CH_4/AIR MIXTURES @ 1873°K

Firing Rate: 20.04 l/min

			NO_x Concentration (PPM)			
Axial Distance (cm)	0.127	0.635	1.27	1.90	2.54	8.13
% Stoich. Air:						
144.3	8	7	6	7	5	8
117.0	14	15	16	18	11	16
97.8	30	32	34	38	29	38
83.5	41	35	36	38	34	43
72.7	33	30	38	41	15	41
64.0	0	0	0	1	6	2
57.0		0	0			

NO_x CONCENTRATION PROFILES CENTERLINE OF THE ADIABATIC STIRRED COMBUSTOR CH_4/AIR MIXTURES @ VARIOUS TEMPERATURES

Firing Rate: 13.78 l/min
Axial Distance: 2.54 cm.

		NO_x Concentration (PPM)		
% Stoich. Air	1723°K	1813°K	1873°K	2073°K[(a)]
405		4		4
314		3		5
254		3		8
212		3		16
182		5		33
158		9		68
139		16		115
124		26	18	170
112	30		33	170
102	37		37	
93	38		34	
80	13		4	
69	3			

(a) axial distance = 15.11 cm.

FIGURE 2-10

NO_x CONCENTRATION PROFILES IN THE ASC WITH C_3H_8/AIR MIXTURES AT 1873°K

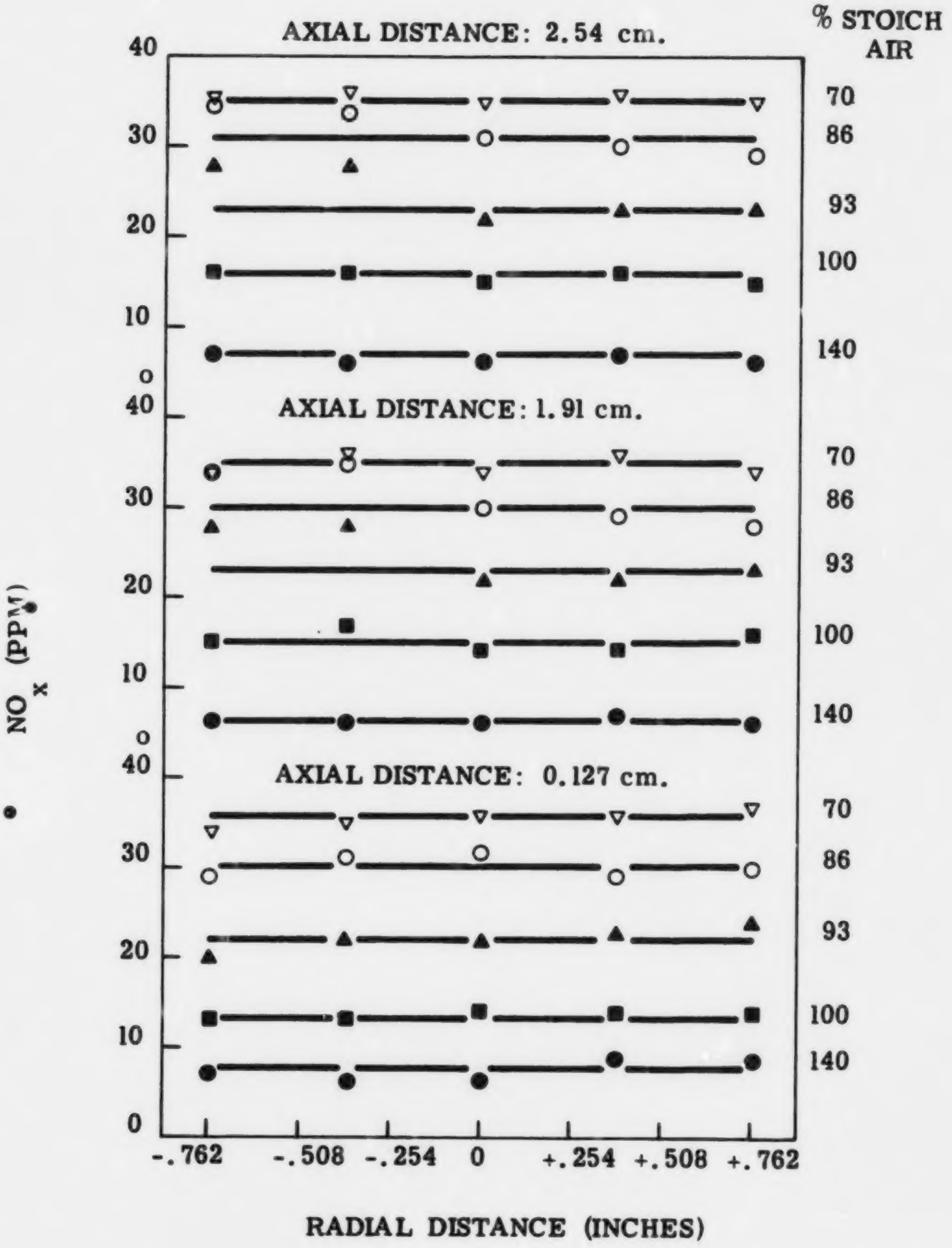

FIGURE 2-11

NO_x PROFILES IN THE ASC FOR C_3H_8/AIR AND CH_4/AIR MIXTURES
1873°K AS A FUNCTION OF AXIAL DISTANCE

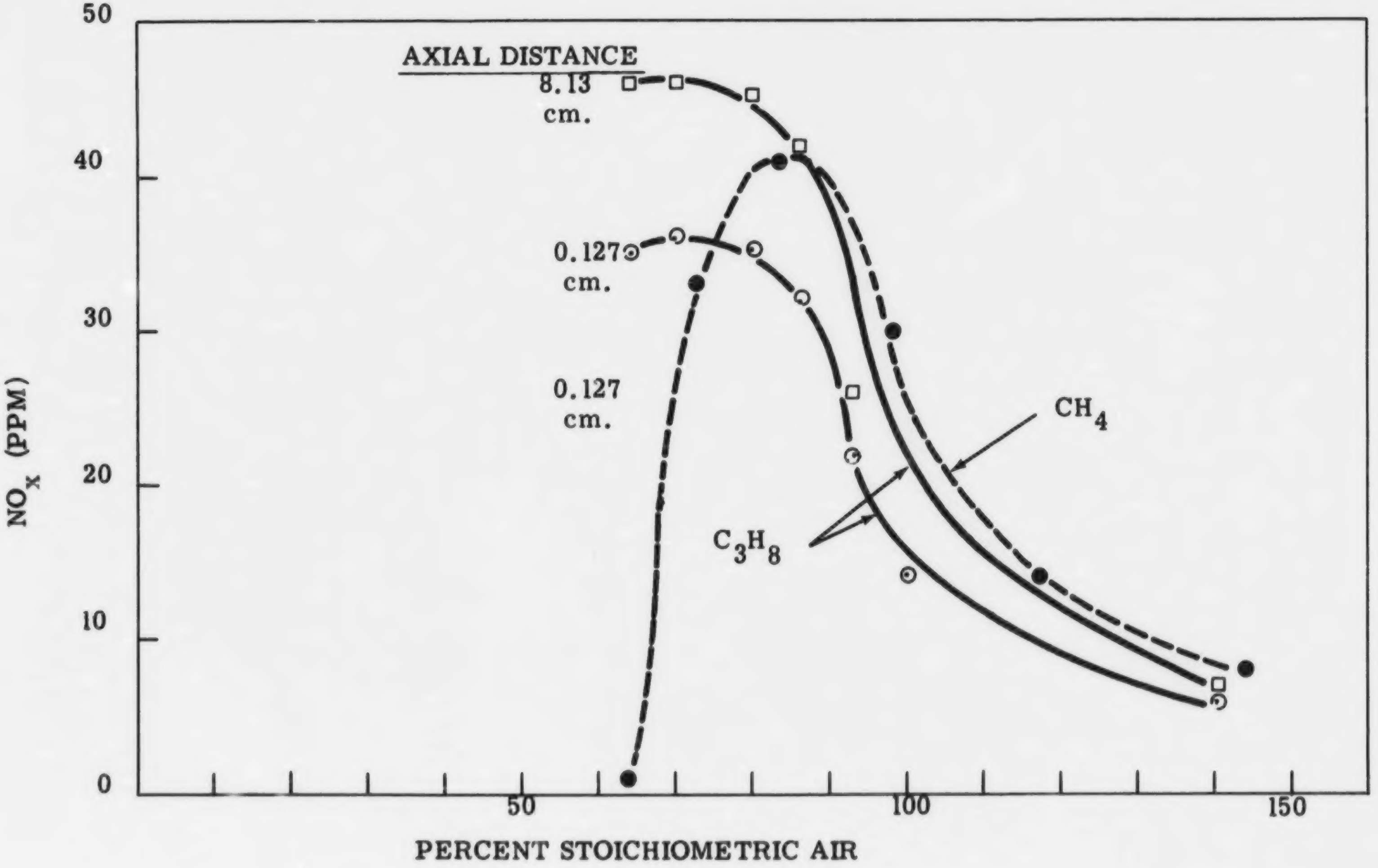

TABLE 2-8

Adiabatic Stirred Combustor Run Identification for Chemical Species Concentration Profiles

CH_4/Air Mixtures

Run #	Firing Rate 1/min.	Wall Temperature (°K)
340	13.78	2073
341	13.78	1813
343	13.78	1873
344	13.78	1873
347	13.78	1723
362	20.04	1873
363	20.04	1873
379	14.60	1998
380	14.60	2047
381	14.60	2226
382	7.02	2226
383	13.92	2226

For C_3H_8/Air Mixtures

Run #	Firing Rate 1/min.	Wall Temperature (°K)
348	15.14	1873
349	15.14	1873
350	15.14	1873
351	16.89	1873
352	16.89	1873
353	16.89	1873
354	16.89	1873
355	16.89	1873
356	16.89	1873
357	16.89	1873
358	16.89	1873
359	16.89	1873
360	16.89	1873

2.9.3 Combustion Parameter Variation in the ASC

Figure 2-12 is the test matrix that was followed to generate the combustion species concentration profiles in the ASC. Changes in firing rate (air flow rate), air preheat temperature and molecular fuel composition were the three variables that were selected for study. The run numbers inside the box of the matrix identifies the computer print-out data sheet for that particular set of variables, which appears in the Appendix. The NO_x concentration profiles for each of the runs are also tabulated as functions of radial and axial dimensions.

2.9.3.1 Reduced Firing Rate and Preheat Effects

The effects of firing rate on NO_x formation under adiabatic conditions for CH_4/Air mixtures are shown in Tables 2-9 and 2-10. In addition, the data from Table 2-9 are plotted in Figure 2-13 in terms of residence times, which were computed from air flow rate and temperature data. The residence times are extrapolated (indicated by dashed line) for lines greater than 152 milliseconds which corresponds to an axial location of 25.4 cm. The plug flow zone was 43.18 cm. long and corresponds to a residence time of about 258 milliseconds at 2073°K for an air flow rate of 7.02 l/min.

The data plotted in Figure 2-13 show that the temperature as well as the residence time have strong effects on NO_x formation. At both 2073°K (121% stoichiometric air) and 2226°K (100% stoichiometric air) doubling the residence times produced a two-fold increase in NO_x concentration. However, the slope of the curve at 100% stoichiometric air and 2226°K was significantly steeper than that at 121% stoichiometric air and 2073°K, even though the oxygen concentration was lower. For a residence time of 100 milliseconds, the corresponding NO_x concentrations at 2226°K and 2073°K are 950 ppm and 300 ppm, respectively. It appears, therefore, that within this range temperature effects can be more important on NO_x formation than residence time and oxygen concentration.

Figure 2-14 shows the effects of air preheat at a near-constant mixture ratio (132% vs 126% stoichiometric air) of CH_4/air with a firing rate of 14.6 l/min. The two-fold increase in NO_x concentration for a temperature increase of 75°K again indicates the importance of temperature for NO_x formation in the post-flame zone.

Tables 2-11 and 2-12 compare the effect of firing rate on NO_x in the H_2/air system at a constant temperature of 2170°K. These data are similar to the CH_4/air combustion results, in that both fuels exhibit the same residence time effects at large distances from the face of the stirred zone. Decreasing the residence time by one-half decreased the NO_x by a factor of two. In both the H2/Air and CH4/Air cases, residence time effects in the vicinity of the face of the adiabatic reactor seemed to be less important than those at greater axial distances and hence larger residence times. Therefore, conventional NO_x formation processes appear to prevail.

FIGURE 2-12

ADIABATIC STIRRED COMBUSTOR
TEST MATRIX AND
RUN IDENTIFICATION

		Methane			Carbon Monoxide & Hydrogen			Hydrogen		
		80% Stoich Air	100% Stoich Air	125% Stoich Air	50% Stoich Air	140% Stoich Air	160% Stoich Air	60% Stoich Air	120% Stoich Air	130% Stoich Air
Normal Firing Rate	298°K Preheat	Run 380	Run 381	Run 379	Runs 392 393	Run 391	Run 390	Run 386	Run 387	Run 389
	423°K Preheat			Run 385						
Reduced Firing Rate	298°K Preheat		Run 382						Run 388	
	423°K Preheat			Run 384						

TABLE 2-9

EFFECT OF FIRING RATE ON NO_x CONCENTRATION PROFILES
CENTERLINE OF THE ADIABATIC COMBUSTOR
CH_4/AIR MIXTURES

NO_x CONCENTRATION (PPM)
Temperature: 2226°K (~/100% Stoich Air)

Axial Distance (cm)	25.4	7.62	2.54	1.27	.635	.127
Firing Rate (l/min)						
CH_4 14.60	860	115	45	37	35	28
7.02	1350	110	51	42	42	41

2073°K CH_4-Air 121% Stoich Air

Axial Distance (cm)	25.4	7.62	2.54	1.27	.635	.127
Firing Rate (l/min)						
7.02	490	58	36	29	27	24
13.92	245	52	29	24	27	18

TABLE 2-10

EFFECT OF MIXTURE RATIO ON NO_x CONCENTRATION PROFILES CENTERLINE OF THE ADIABATIC STIRRED COMBUSTOR CH_4/AIR MIXTURES

Firing Rate: 14.6 l/min.

Axial Distance (cm)	25.4	7.62	2.54	1.27	.635	.127
Percent Stoich. Air	NO_x Concentration (PPM)					
132 (1998°K)	115	34	17	18	17	11
105 (2226°K)	860	115	45	37	35	28
84 (2097°K)	77	63	47	30	39	32
Air Preheated to 170°C						
126 (2073°K)	245	52	29	24	21	18

CENTERLINE NO_x CONCENTRATIONS IN CH_4/AIR AS A FUNCTION OF RESIDENCE TIME AND PERCENT STOICHIOMETRIC AIR IN ADIABATIC STIRRED COMBUSTOR

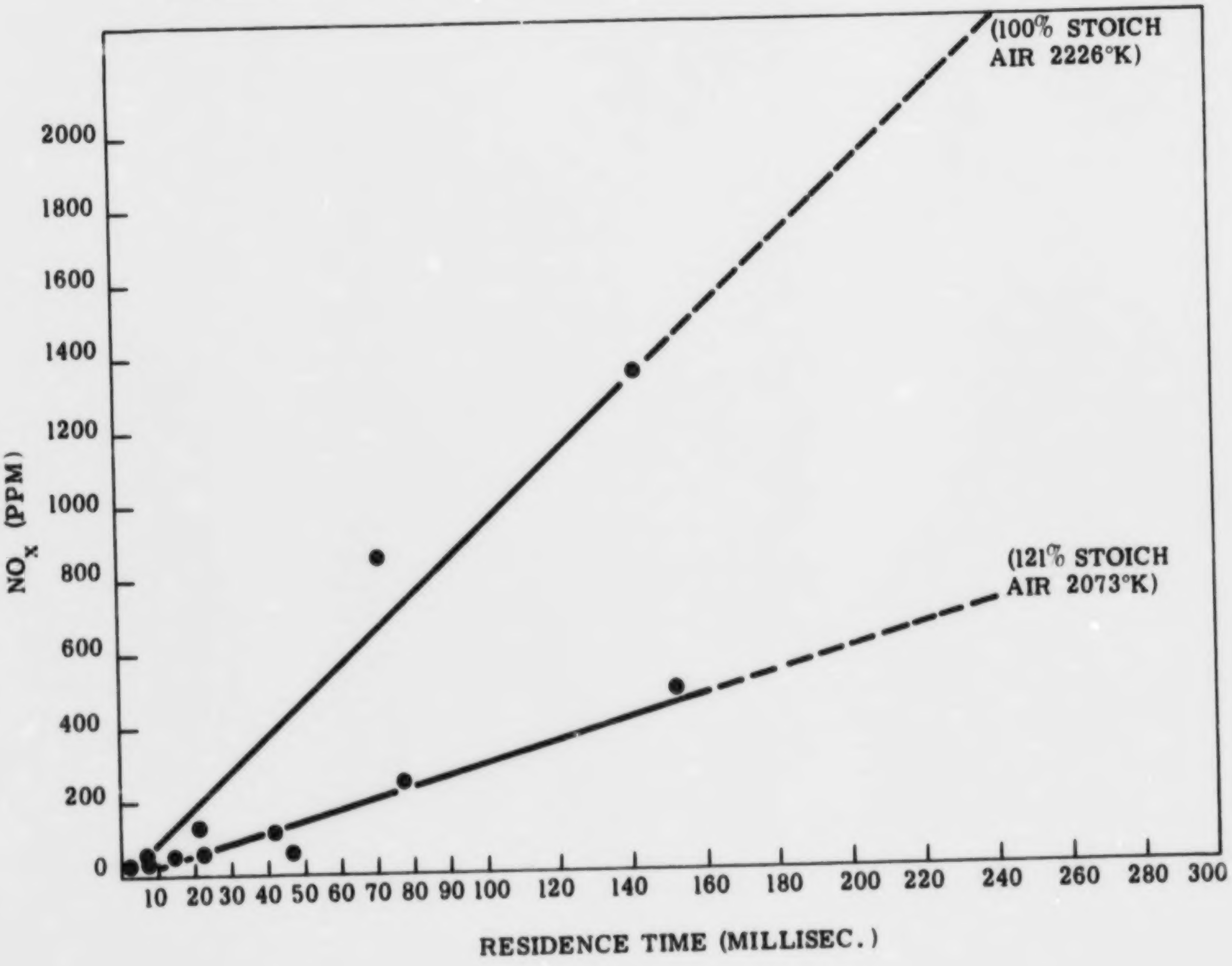

FIGURE 2-14

CENTERLINE NO_x IN CH_4/AIR ASC AS A FUNCTION OF AXIAL DISTANCE

FIRING RATE: 14.603 l/MIN.

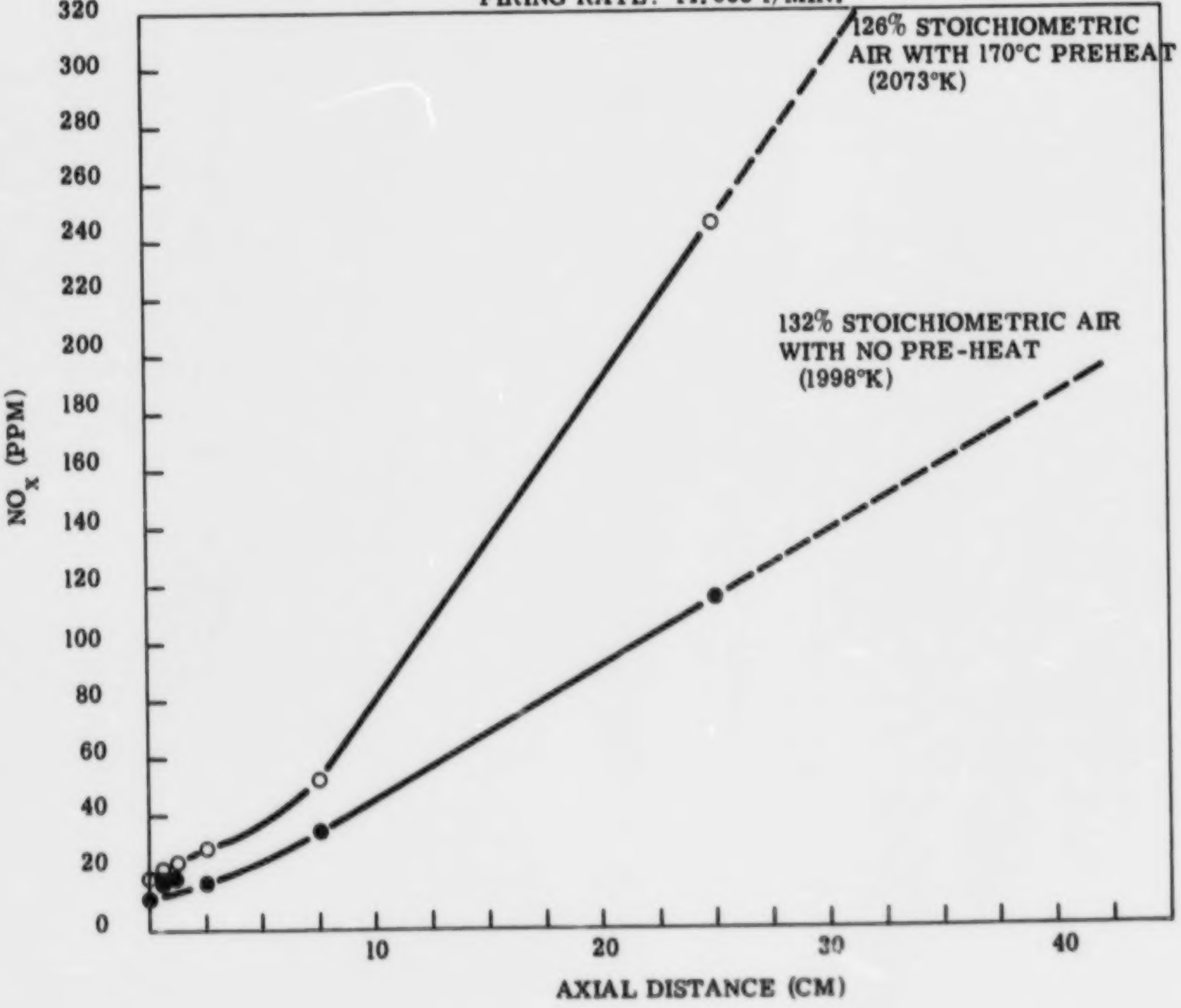

TABLE 2-11

EFFECT OF MIXTURE RATIOS ON NO_x CONCENTRATION PROFILES CENTERLINE OF THE ADIABATIC STIRRED COMBUSTOR H_2/AIR MIXTURES

Firing Rate: 13.92 1/min.

Axial Distance (cm)	25.4	7.62	2.54	1.27	.635	.127
Percent Stoich. Air			NO_x Concentration (PPM)			
60 (2183°K)	1	1	1	1	1	1
120 (2170°K)	680	44	18	14	11	10
130 (1958°K)	45	17	10	9	8	7

TABLE 2-12

EFFECT OF FIRING RATE ON NO_x CONCENTRATION PROFILES CENTERLINE OF THE ADIABATIC STIRRED COMBUSTOR H_2/AIR MIXTURES

		Percent Stoich. Air: 117-120 (T = 2170°K)				
Axial Distance (cm)	25.4	7.62	2.54	1.27	0.635	0.127
Firing Rate (1/min)						
13.92	620	34	13	10	8	7
6.96	1150	36	13	9	8	8

EFFECT OF MIXTURE RATIO ON NO_x CONCENTRATION PROFILES CENTERLINE OF THE ADIABATIC STIRRED COMBUSTOR CO/H_2/AIR MIXTURES

Firing Rate: 14.60 1/min.

Axial Distance (cm)	25.4	7.62	2.54	1.27	0.635	0.127	(% H_2)
Percent Stoich. Air			NO_x Concentration (PPM)				
139 (2009°K)	950	160	45	27	19	17	17
125 (2150°K)	930	175	50	33	25	21	15
48 (2150°K)	46	31	19	14	15	14	5
51 (2150°K)	245	160	43	27	17	11	0

2.9.3.2 Variation of NO_x Concentration with Fuel Type

To gain a better understanding of the effects of molecular fuel structure on NO_x formation under adiabatic conditions a series of experiments were conducted with H_2-air and CO-H_2-air mixtures. The walls of the ASC were maintained at theoretical adiabatic flame temperatures for fuel lean and fuel rich mixtures. The resulting NO_x concentration profiles which were obtained on the centerline of the combustor at various axial distances from the face of the stirred combustor are summarized in Tables 2-11 and 2-12.

The data showed that under rich conditions and at a firing rate of 13.9-14.6 l/min., the NO_x concentrations 0.127 cm. from the face of the stirred combustor were 1 ppm for H_2, 11 ppm for CO and 14 ppm for CO with 5% H_2. Measurements 25 cm. from the surface of the stirred combustor showed that no change in NO_x concentration occurred for the fuel rich H_2-air mixture while the NO_x concentrations increased in the case of CO/H_2 and in the case of CO without added hydrogen. This was true even though the hydrogen/air mixture had an adiabatic flame temperature 33°K higher than either one of the CO-H_2 or CO-air mixtures; the residual oxygen concentration offers an explanation for these observations. The oxygen burnout is slower with less hydrogen. Under fuel lean conditions where 15% H_2 was added to CO, the NO_x concentration near the face of the burner was 21 ppm while for the pure H_2-air mixture, 10 ppm NO_x was measured. At a distance of 25 cm. from the face of the combustor, at similar stoichiometries and temperatures, the 15% H_2-CO mixture produced 930 ppm NO_x and the pure H_2-air mixture resulted in 680 ppm NO_x.

As will be shown in the next section, the theoretical calculations indicated that for a stirred reactor operating between 50 and 150% stoichiometric air, the NO_x concentrations increased as H_2 addition to CO was increased from 1 to 10%. The NO_x concentration, however, reached a maximum and decreased as more H_2 was added reaching significantly lower values for fuel rich conditions in the pure H_2-air system (see Section 3). As indicated above, the NO_x concentrations measured at a distance of 25 cm. from the face of the stirred combustor were greatest for the rich CO-air system compared to the H_2-air or 5% H_2-CO-air mixtures because of higher residual O_2 concentrations.

3. CHEMICAL KINETICS CALCULATIONS

The theoretical calculations conducted during this phase of the program concentrated on stirred reactor calculations for methane, carbon monoxide and hydrogen/air combustion. The purpose of these calculations was primarily to investigate the chemical mechanism for the formation of NO_x and other pollutants in methane-air combustion and also to obtain comparisons with experimental data for methane, carbon monoxide and hydrogen air combustion obtained under conditions as free as possible from fluid mechanical, diffusion and heat transfer limitations. Since even flat flame experiments conducted at atmospheric pressure were found to be strongly influenced by diffusional effects in Phase I of this study, the Adiabatic Stirred Combustor experiments (described in Section 2 of this report) were used as the basis for comparison. In the approach to this series of calculations, consideration was given to all unimolecular and bimolecular reactions for 25 species of potential importance for methane/air combustion at one atmosphere, between 1500 and 2500 K. The species and reaction selection as well as the results of the calculations are discussed in this section. Further detail on the procedures used will be found in Reference 3-1.

3.1 Methodology of Kinetics Calculations

While a common approach to studies of kinetic mechanism is to postulate reaction steps and revise as few steps or rates as possible to fit the experimental observations, a detailed, objective approach was used in this study. The technique used involved starting the procedure with species selection. Previous studies and experience, along with thermochemical considerations, were used to select species for inclusion in the mechanism. Next, all possible unimolecular and bimolecular reactions were constructed by use of a computer code which listed these reactions in the filing order of the JANNAF Tables. These unimolecular and bimolecular reactions were then evaluated for potential importance to methane-air combustion under the conditions of interest (one atmosphere, 1500-2500 K, 80-125% stoichiometric air). As a result of this evaluation, about two-thirds of the reactions were found unlikely to be important on the basis of stereochemistry, thermochemistry or on the basis of relative rates of competing reactions with the same species.

3-1 Engleman, V. S., "Survey and Evaluation of Kinetic Data on Reactions in Methane/Air Combustion", Final Report, EPA Contract 68-03-0224, Report No. EPA-600/2-76-003, (January 1976).

This section describes the methodology used in this process for methane/air combustion. It should be carefully noted that these conclusions on the probable relative importance of the reactions considered pertain only to the chemical and physical constraints of the system (methane/air combustion, 80-125% stoichiometric air, at one atmosphere between 1500 and 2500 K). Thus, if one were considering a reaction system at pressures significantly above or below one atmosphere, or at temperatures below 1500 K or above 2500 K, or at mixture ratios below 80% or above 125% stoichiometric air, a reevaluation of species, reaction importance and reaction rates would be required.* In addition, if one were considering combustion of higher hydrocarbons, combustion of oxygenated hydrocarbons or conversion of nitrogen-containing species in combustion, it would be necessary to consider additional species and reactions, and to re-evaluate the relative importance of reactions considered.

3.1.1 Species Selection

This study was limited to methane/air combustion with subsets of carbon monoxide/air and hydrogen/air combustion. As such it was desirable to minimize the number of species considered to keep the task to a tractable size and yet not eliminate potentially important species. Species were selected on thermochemical grounds with special consideration given to species postulated to play a role in methane/air combustion and pollutant formation. The primary list of 25 species, along with the considerations that entered into their selection, and the JANNAF Tables reference for thermochemical data are given in Table 3-1.

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* Note that the temperature limitations have definite implications for the ignition process. Since ignition for plug flow reactors is likely to occur below 1500°K, additional consideration may be required for ignition calculations. The pre-screened set may be used as a starting point for ignition calculations but special attention should be paid to the results to see if they make sense chemically.

Table 3-1

Primary Species for Methane-Air Combustion

Species	Log KP at 2000K	Considerations	JANNAF Reference
CH	-10	hydrocarbon radical	12/67
CHN	-2	possible role in prompt NO	12/69
CHO	+1	stable radical	12/70
CH_2	-7	hydrocarbon radical	12/72
CH_2O	+1	combustion intermediate	3/61
CH_3	+5	hydrocarbon radical	6/69
CH_3O	-6	possible role in ignition	constructed from CH_3F 12/63
CH_4	-3	starting material	3/61
CN	-6	possible role in prompt NO	6/69
CO	+7	combustion product	3/61
CO_2	+10	combustion product	9/65
H	-3	combustion intermediate	9/65
NH	-9	possible role in prompt NO	7/72
HNO	-5	possible role in prompt NO	3/63
HO	0	combustion intermediate	12/70
HO_2	-3	combustion intermediate	3/64
H_2	0	combustion product	3/61
H_2O	+4	combustion product	3/61
N	-9	important role NO formation	3/61
NO	-2	of prime interest	6/63
NO_2	-4	oxidation of NO	9/64
N_2	0	starting material	3/61
N_2O	-6	possible role NO formation	12/64
O	-3	combustion intermediate	6/62
O_2	0	starting material	3/61

3.1.2 Reaction List Compilation

By use of a computer code developed for this study, all mathematically possible unimolecular and bimolecular reactions were assembled for the 25 species considered. The magnitude of the problem can be grasped when it is noted that these 25 species result in a list of 322 reactions. The exponential growth of the number of reactions can be appreciated from the fact that if the species list is expanded to around 40 species, over 1000 reactions are mathematically possible. Since these reaction lists are strictly mathematical constructions, and contain both elementary reactions and overall reaction steps, further evaluation of the likelihood of any of these reactions in a physical or a chemical sense is required.

3.1.3 Reactions of Potential Importance

The relative importance of chemical reactions in a mechanism depends, to a certain extent, on the goals of the calculation. For the case of methane/air combustion and pollutant formation, reactions of importance for NO_x formation may be totally unimportant for heat release. However, many of the combustion reactions are extremely important for NO_x formation. Starting with the list of all mathematically possible unimolecular and bimolecular reactions, non-elementary reactions were eliminated. Since activation energy strongly influences reaction rate, (at 2000 K, 40 kcal/mole is equivalent to four orders of magnitude in the rate and 100 kcal/mole is equivalent to ten orders of magnitude) thermochemical considerations were taken into account. Alternate paths and (in a gross sense) relative concentrations were also considered. Under specific circumstances a low energy path between intermediates could be unimportant because of a more favorable alternate path. In other cases a high energy path may be the only alternative for a reaction of important species, e.g.,

$$N_2 + O = NO + N \qquad \text{endothermic 75 kcal}$$

Also, for some situations a given reaction will be unimportant because alternate paths are available with higher concentration intermediates.

In the process of reaction pre-screening on stereochemical and thermochemical grounds, while there was a major incentive to minimize the number of reactions retained, marginal reactions were retained to allow any further eliminations to be done after detailed calculations. Caution was exercised to avoid elimination of endothermic reactions with high concentration species unless alternate paths were clearly dominant.

The evaluation of the probable relative importance of all possible unimolecular and bimolecular reactions of these 25 species under conditions of interest is given in Appendix B. The original list of 322 reactions for 25 species was thus reduced to 101 reactions of potential importance.

3.1.4 Rates for Reactions Used in Kinetics Calculations

The rates used in the present calculations for the reactions considered to be of potential importance under the conditions of interest were based on a critical survey of the literature and on estimates for rates of reactions which were not found in the literature. A detailed account of survey and evaluation will be found in reference 3-1. The rates used in the present study (given in Table 3-2) were based on recommended rates as of December 1974, while the rates given in Reference 3-1 are updated to July 1975. The reactions are written in the filing order for the kinetics survey. The rates for the forward direction are indicated as KF and the rates for the reverse direction of the reaction written are indicated as KR. The values of log A, B, and C are given in the table where rate = $10^{\log A} T^{B} e^{-(C/RT)}$.

3.1.5 Calculations Performed

As indicated earlier, calculations were performed for a stirred reactor system. Calculations were accomplished with the GKAP code, developed by Ultrasystems and modified under contract to EPA (68-02-0220) for the purpose of calculations of combustion/pollutant formation. Primary attention was focused on stirred reactor calculations of methane/air combustion using the 101 reactions selected as indicated previously. In addition, calculations were performed for hydrogen/air and carbon monoxide/air combustion. Modified combustion runs (preheat, water addition and flue gas recirculation) were performed for methane/air combustion.

3.2 Results of Kinetics Calculations

The chemical kinetics calculations performed in this study were aimed at the understanding of the chemistry of combustion and pollutant formation (with special attention to NO_x formation) under conditions where fluid mechanics, species diffusion and heat transfer were not controlling. As a result, the perfectly stirred reactor system was used as the model system to be studied since such a system can also be approached experimentally. Plug flow calculations such as were accomplished in Phase I of this study were not pursued since the calculations themselves indicated steep concentration gradients that would require the inclusion of diffusion effects and introduce undesirable uncertainty in a study aimed at defining chemical effects.

A further advantage to the use of a stirred reactor system for this study is derived from the uniform species and temperature distribution in a perfectly stirred reactor. This fact greatly simplifies the theoretical analysis of the chemical system and allows simpler comparisons with the experimental work. Since the chemical system being investigated in the stirred reactor is operating at a single steady condition, the reactions of importance do not vary from point to point within the reactor or from moment to moment at a given mode of operation.

Table 3-2

		LOG A	B		C
RX 1 CH +CHN =CH2 +CN ,	KR=	3.00E12,	0.00	,	5.0
FX 9 CH +CH4 =CH2 +CH3 ,	KF=	2.50E11,	0.70	,	6.0
FX 10 CH +CO2 =CHO +CO ,	KF=	1.00E10,	0.50	,	6.0
FX 20 CH +HO =CHO +H ,	KF=	5.00E11,	0.50	,	10.0
FX 25 CH +HO2 =CH2 +O2 ,	KF=	1.00E10,	0.50	,	15.0
RX 29 CH +H2 =CH2 +H ,	KR=	3.00E11,	0.70	,	26.0
RX 32 CH +H2O =CH2 +HO ,	KR=	5.00E11,	0.50	,	6.0
FX 38 CH +NO =CHN +O ,	KF=	2.00E12,	0.00	,	0.0
FX 39 CH +NO =CHO +N ,	KF=	1.50E13,	0.00	,	10.0
FX 47 CH +N2 =CHN +N ,	KF=	2.00E13,	0.00	,	48.0
FX 48 CH +N2 =CN +HN ,	KF=	3.00E14,	0.00	,	92.0
FX 53 CH +O =CO +H ,	KF=	5.00E11,	0.50	,	0.0
FX 54 CH +O2 =CHO +O ,	KF=	5.00E11,	0.50	,	6.0
RX 59 CHN +CH2 =CH3 +CN ,	KR=	1.00E11,	0.70	,	3.0
RX 61 CHN +CH3 =CH4 +CN ,	KR=	3.00E11,	0.70	,	5.0
RX 64 CHN +H =CN +H2 ,	KR=	3.00E12,	0.00	,	5.0
RX 65 CHN +HN =CH2 +N2 ,	KR=	1.00E14,	0.00	,	70.0
FX 71 CHN +HO =CN +H2O ,	KF=	2.00E11,	0.60	,	5.0
RX 85 CHN +O =CHO +N ,	KR=	1.00E14,	0.00	,	0.0
RX 86 CHN +O =CN +HO ,	KR=	3.00E12,	0.00	,	3.0
RX 92*CHO =CO +H ,	KR=	1.50E20,	-1.50	,	0.0
FX 94 CHO +CHO =CH2O+CO ,	KF=	1.50E11,	0.50	,	0.0
FX 95 CHO +CH2 =CH3 +CO ,	KF=	3.00E10,	0.70	,	1.0
RX 98 CHO +CH3 =CH2 +CH2O,	KR=	3.00E10,	0.50	,	6.0
FX 99 CHO +CH3 =CH4 +CO ,	KF=	3.00E11,	0.50	,	0.0

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* Dissociation-recombination reaction; third-body, M, participates but is not shown.

Table 3-2 (Continued)

			LOG A	B	C
RX103	CHO +CH4 =CH2O+CH3 ,	KR=	1.00E10,	0.50 ,	6.0
RX104	CHO +H =CH2 +O ,	KR=	5.00E11,	0.50 ,	4.0
FX106	CHO +H =CO +H2 ,	KF=	1.50E12,	0.50 ,	0.0
RX113	CHO +HO =CH2O+O ,	KR=	1.00E11,	1.00 ,	3.5
FX114	CHO +HO =CO +H2O ,	KF=	3.00E10,	1.00 ,	0.0
FX116	CHO +HO2 =CH2O+O2 ,	KF=	1.00E14,	0.00 ,	3.0
RX119	CHO +H2 =CH2O+H ,	KR=	1.25E10,	1.00 ,	3.2
RX123	CHO +H2O =CH2O+HO ,	KR=	3.00E10,	1.00 ,	0.0
FX127	CHO +N =CO +HN ,	KF=	2.00E11,	0.50 ,	2.0
FX129	CHO +NO =CO +HNO ,	KF=	2.00E11,	0.50 ,	2.0
FX133	CHO +O =CO +HO ,	KF=	3.00E11,	1.00 ,	0.5
FX134	CHO +O =CO2 +H ,	KF=	3.00E11,	0.00 ,	0.0
FX135	CHO +O2 =CO +HO2 ,	KF=	1.50E12,	0.00 ,	7.0
FX139	CH2 +CH4 =CH3 +CH3 ,	KF=	1.00E12,	0. ,	12.
FX146	CH2 +HO =CH2O+H ,	KF=	1.00E13,	0. ,	5.
FX147	CH2 +HO =CH3 +O ,	KF=	5.00E11,	0.5 ,	6.
RX150	CH2 +HO2 =CH3 +O2 ,	KR=	3.00E12,	0. ,	69.5
FX152	CH2 +H2 =CH3 +H ,	KF=	3.00E12,	0. ,	7.
RX155	CH2 +H2O =CH3 +HO ,	KR=	6.30E10,	0.7 ,	2.
FX159	CH2 +NO =CH2O+N ,	KF=	1.50E12,	0. ,	7.
FX165	CH2 +O2 =CH2O+O ,	KF=	5.00E11,	0.5 ,	7.
RX171	CH2O+H =CH3 +O ,	KR=	5.00E13,	0. ,	0.
RX172*	CH2O+H =CH3O ,	KR=	4.00E40,	-7.5 ,	22.6
RX174	CH2O+HN =CH3O+N ,	KR=	1.00E14,	0. ,	0.
RX177	CH2O+HO =CH3 +O2 ,	KR=	3.00E13,	0. ,	20.

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* Dissociation-recombination reaction; third-body, M, participates but is not shown.

Table 3-2 (Continued)

			LOG A	B	C
RX178	CH2O+HO =CH3O+O	KR=	1.00E14	0.	0.
RX179	CH2O+HO2 =CH3O+O2	KR=	1.00E12	0.	6.
RX181	CH2O+H2 =CH3O+H	KR=	1.00E14	0.	0.
RX184	CH2O+H2O =CH3O+HO	KR=	3.00E13	0.	0.
RX191*	CH3 +H =CH4	KR=	2.00E17	0.	87.5
FX195	CH3 +HO =CH3O+H	KF=	6.30E12	0.	0.
RX196	CH3 +HO =CH4 +O	KR=	2.00E13	0.	9.
FX196	CH3 +HO2 =CH4 +O2	KF=	1.00E11	0.5	6.
RX199	CH3 +H2 =CH4 +H	KR=	6.30E13	0.	11.9
RX201	CH3 +H2O =CH4 +HO	KR=	3.00E13	0.	5.
FX206	CH3 +O2 =CH3O+O	KF=	3.00E12	0.	30.
FX216	CN +NO =CO +N2	KF=	3.00E11	0.	0.
FX219	CN +O =CO +N	KF=	1.00E12	0.	0.
FX220	CN +O2 =CO +NO	KF=	3.00E11	0.	0.
FX223	CO +HO =CO2 +H	KF=	1.50E07	1.3	-0.76
RX229*	CO +O =CO2	KR=	1.00E15	0.	100.
FX230	CO +O2 =CO2 +O	KF=	3.00E12	0.	50.
RX231*	H +H =H2	KR=	2.00E14	0.	96.
FX233	H +HNO =HN +HO	KF=	2.00E11	0.5	23.
FX234	H +HNO =H2 +NO	KF=	1.00E13	0.	2.5
FX236	H +HO =H2 +O	KF=	8.00E09	1.	7.
FX237*	H +HO =H2O	KF=	2.00E22	-2.	0.
FX238	H +HO2 =HO +HO	KF=	2.50E14	0.	1.9
FX239	H +HO2 =H2 +O2	KF=	2.50E13	0.	0.7
RX241	H +H2O =HO +H2	KR=	2.50E13	0.	5.2

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* Dissociation-recombination reaction; third-body, M, participates but is not shown.

Table 3-2 (Continued)

						LOG A	B	C
RX243	H	+NO	=HN	+O	KR=	6.30E11	0.5	0.
RX245	H	+NO	=HO	+N	KR=	6.30E11	0.5	0.
FX248	H	+NO2	=HO	+NO	KF=	3.00E14	0.	1.5
FX253	H	+N2O	=HO	+N2	KF=	8.00E13	0.	15.
FX254*	H	+O	=HO		KF=	8.00E15	0.	0.
RX255	H	+O2	=HO	+O	KR=	2.50E13	0.	0.
FX256*	H	+O2	=HO2		KF=	2.00E15	0.	1.
FX261	HN	+HO	=H2O	+N	KF=	5.00E11	0.5	2.
RX274	HN	+O2	=HNO	+O	KR=	1.00E11	0.5	7.
FX280	HNO	+HO	=H2O	+NO	KF=	3.00E13	0.	0.
FX286	HNO	+O	=HO	+NO	KF=	5.00E11	0.5	0.
FX291	HO	+HO	=H2O	+O	KF=	6.30E12	0.	1.
FX292	HO	+HO2	=H2O	+O2	KF=	5.00E13	0.	1.
RX295	HO	+NO2	=HO2	+NO	KR=	1.00E13	0.	3.
FX296	HO	+N2O	=HO2	+N2	KF=	3.00E13	0.	15.
FX297*	HO	+O	=HO2		KF=	1.00E17	0.	0.
RX298	HO	+O2	=HO2	+O	KR=	5.00E13	0.	1.
FX305	N	+NO	=N2	+O	KF=	1.60E13	0.	0.
FX307	N	+NO2	=NO	+NO	KF=	4.00E12	0.	0.
FX312	N	+O2	=NO	+O	KF=	6.30E09	1.	6.3
RX315	NO	+NO	=N2O	+O	KR=	1.00E14	0.	28.
RX318*	NO	+O	=NO2		KR=	1.00E16	0.	65.
RX319	NO	+O2	=NO2	+O	KR=	1.00E13	0.	1.
RX320*	N2	+O	=N2O		KR=	5.00E14	0.	58.
RX321	N2	+O2	=N2O	+O	KR=	1.00E14	0.	28.
RX322*	O	+O	=O2		KR=	2.50E18	-1.	118.7

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* Dissociation-recombination reaction; third-body, M, participates but is not shown.

The Phase I study of a nonadiabatic stirred reactor under this contract showed that experimental results of NO_x formation for hydrogen/air combustion (Figure 3-1) and carbon monoxide/air combustion (Figure 3-2) could be modeled by a fairly simple chemical mechanism (Reference 3-2) but that predictions of NO_x formation for the combustion of propane/air in the same combustor seriously underpredicted the results (Figure 3-3). It should be noted that those calculations were not done with the same reaction set being described in this report but by an oversimplified quasi-global mechanism. The results of the present work tend to invalidate the use of such oversimplified approaches to the treatment of detailed mechanisms of coupled kinetic phenomena.

For the present theoretical investigation methane/air, hydrogen/air, and carbon monoxide/air combustion systems were studied for a perfectly stirred reactor operating adiabatically at one atmosphere. The purpose of this investigation was to identify the reactions responsible for NO_x formation in hydrocarbon combustion and to study their influence over a wide range of conditions. In order to investigate the relative importance of reactions in methane/air combustion under conditions from fuel-rich to fuel-lean, the pre-screened set of 101 reaction discussed previously was used as the starting point for the study of methane/air combustion and appropriate subsets were used for the studies of hydrogen/air and carbon monoxide/air combustion. The results of the theoretical calculations will be discussed in this section and the reactions of importance and the comparison of the theoretical calculations with experimental results will be discussed in subsequent sections.

3.2.1 Methane-Air Combustion

The combustion of methane-air in an adiabatic stirred reactor was studied theoretically* for normal combustion between 80 and 125 per cent stoichiometric air and for modified combustion with preheat, flue gas recirculation and water addition. Attention was focused on the reactions that were found to be significant in the mechanism as opposed to the definition of a minimum set of reactions since the latter definition is subject to specific experimental criteria and selection of retention criteria.

The initial calculations for methane/air combustion at 100% stoichiometric air, using the prescreened reaction set, were quite surprising in light of the previous calculations on propane. Rather than underpredicting experimental results by a factor of 4 to 10 as had previously been the case with a quasi-global mechanism (3-2), the predicted NO_x levels were orders of magnitude higher than those found experimentally. The predicted NO_x levels were over 4000 ppm while experimental results were between 10 and 100 ppm. Inspection showed that the reaction responsible for the high NO_x levels was the reaction

$$CH + N_2 \rightarrow HCN + N$$

3-2 V. S. Engleman, W. Bartok, J. P. Longwell and R. B. Edelman, Fourteenth Symposium (International) on Combustion, The Combustion Institute, p. 755 (1973).

* This theoretical system matches the conditions established in the Adiabatic Stirred Combustor in the experimental part of this study.

FIGURE 3-1

COMPARISON BETWEEN EXPERIMENTAL AND CALCULATED NO_x CONCENTRATIONS IN A JET-STIRRED COMBUSTOR (FROM REFERENCE 3-2)

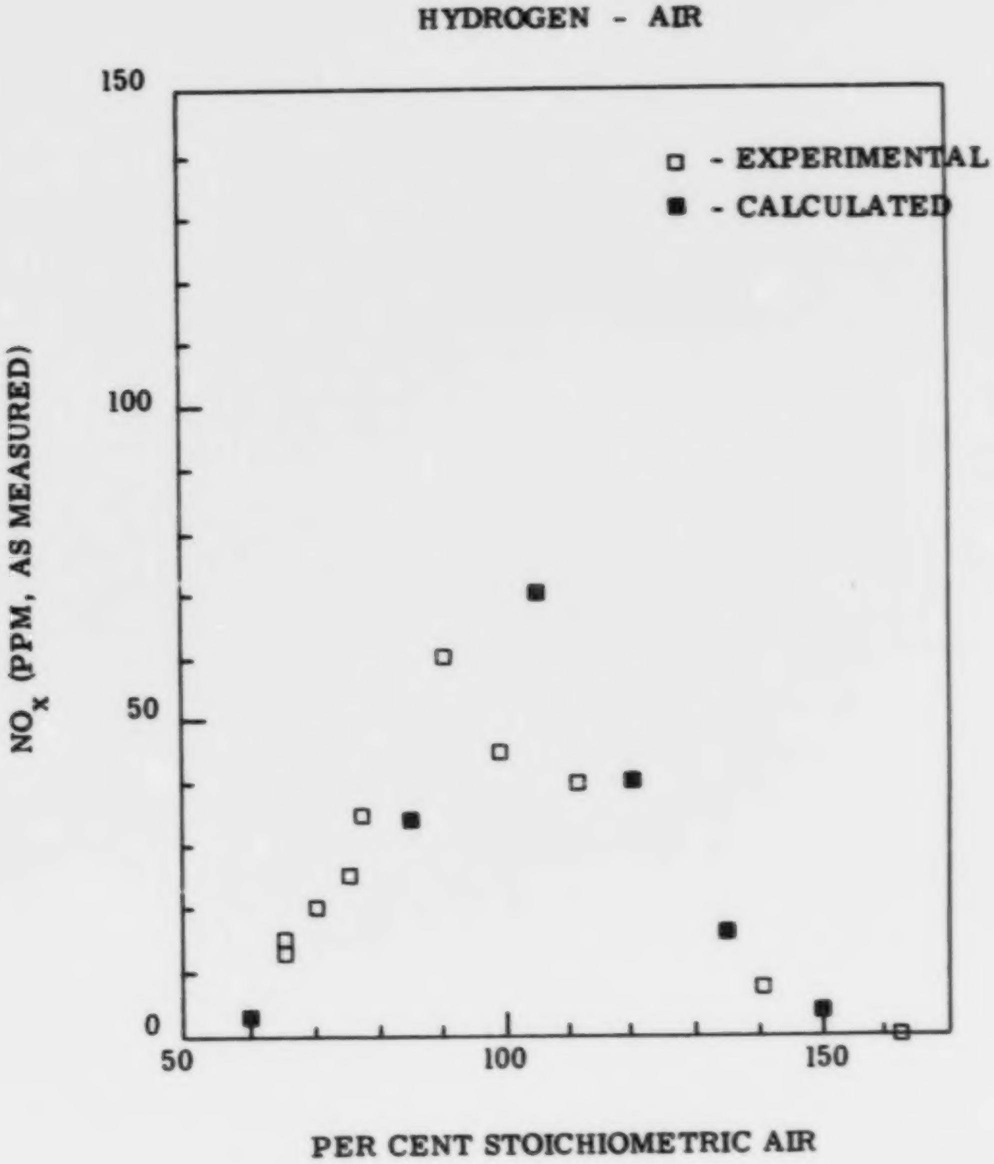


FIGURE 3-2

COMPARISON BETWEEN EXPERIMENTAL AND CALCULATED NO_x CONCENTRATIONS IN A JET-STIRRED COMBUSTOR (FROM REFERENCE 3-2)

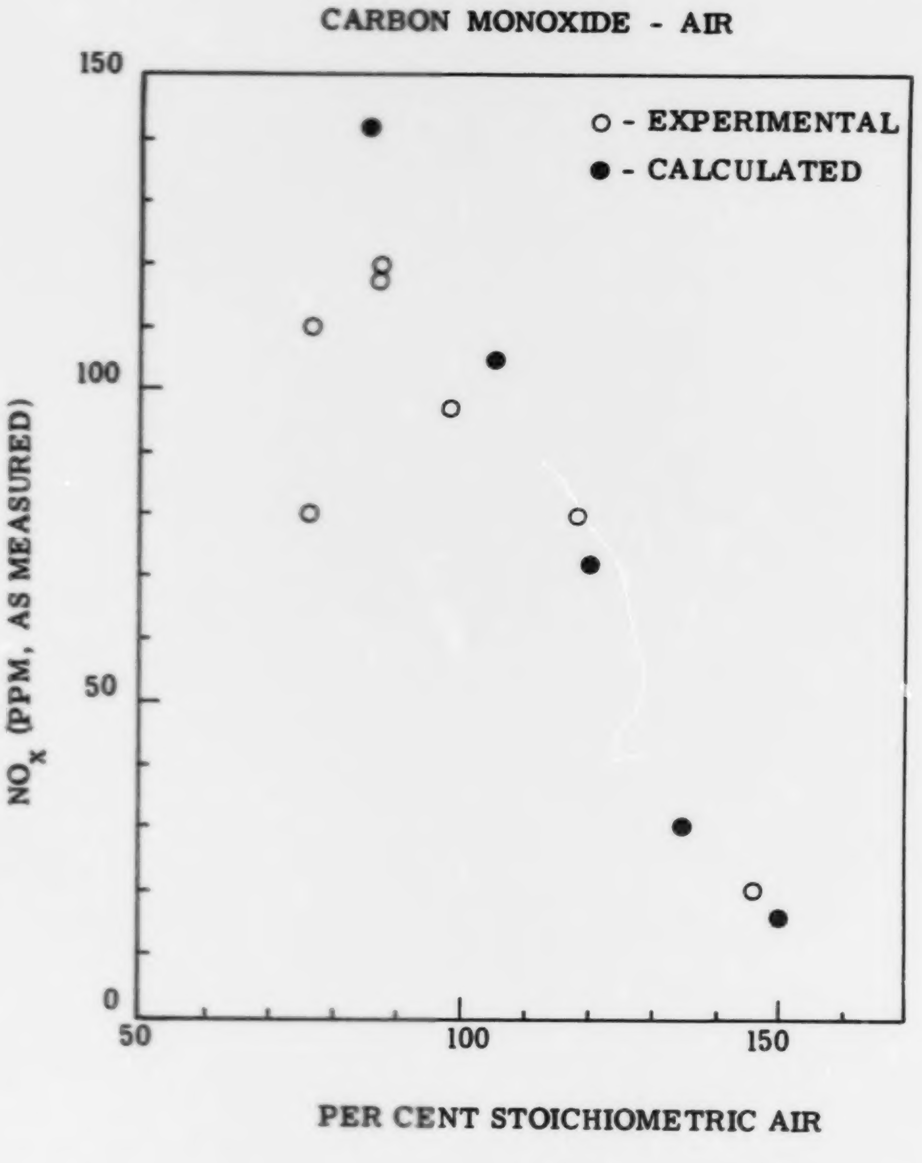
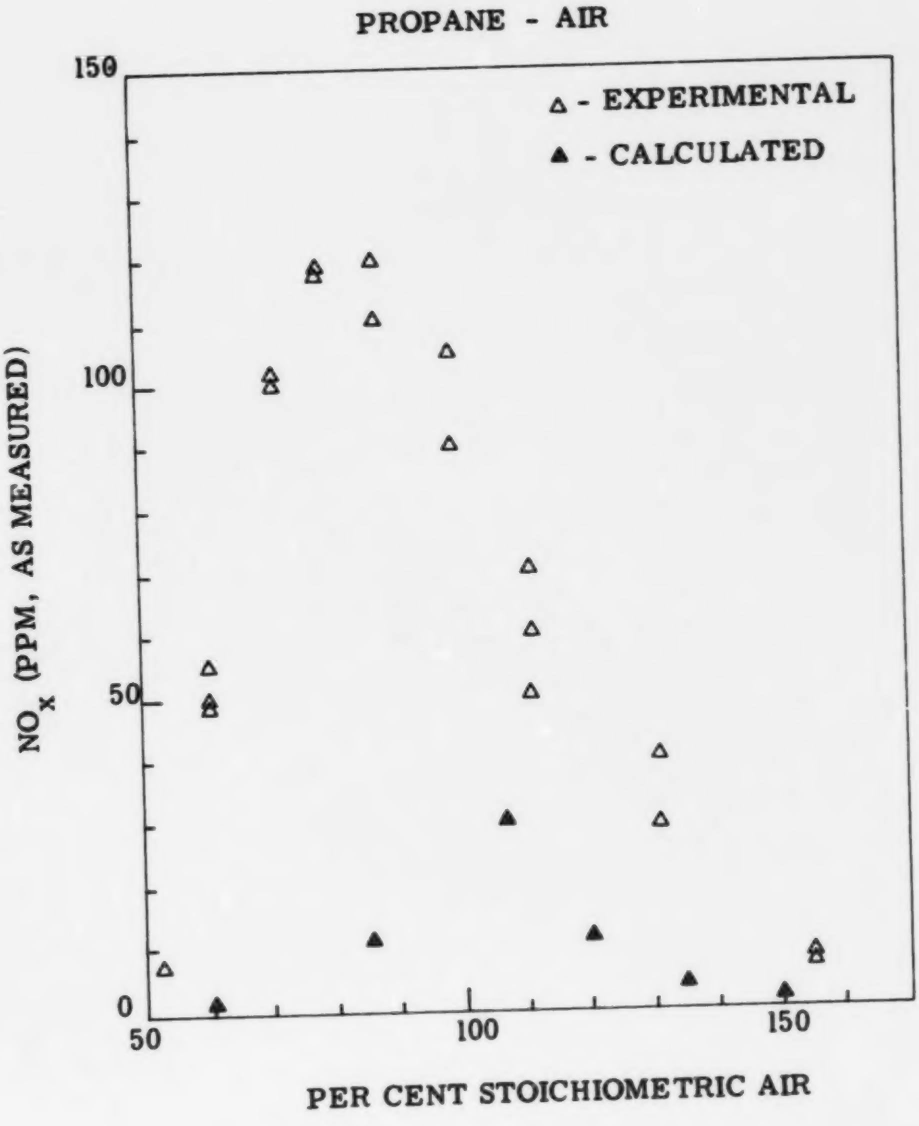


FIGURE 3-3

COMPARISON BETWEEN EXPERIMENTAL AND CALCULATED NO_x CONCENTRATIONS IN A JET-STIRRED COMBUSTOR (FROM REFERENCE 3-2)

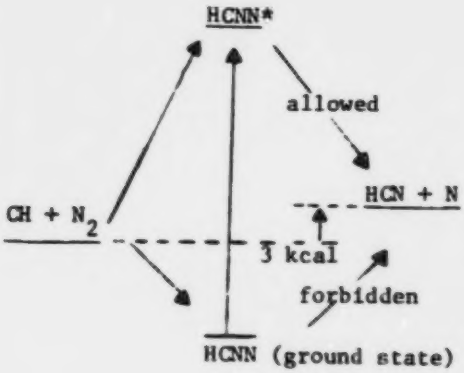


The initially estimated rate coefficient used for this reaction** caused the reaction rate to be so fast that extremely high levels of both HCN (760 ppm) and N (2.7 ppm) were predicted which ultimately resulted in very rapid NO formation. The concentration of N atom was so high, in fact, that a portion of the Zeldovich mechanism was "running backwards".

$$N + NO \rightarrow N_2 + O$$

Such a situation might be considered possible under circumstances where N atoms might be introduced artifically or could be produced in high concentrations from N-containing species, but must be viewed with skepticism for methane-air combustion at 100 per cent stoichiometric air.

In an effort to rectify the situation, the assumed rate of the CH + N_2 reaction was reduced in sequential steps. The rate constant was reduced by one order of magnitude, then two, three and finally three and one-half orders of magnitude to investigate the sensitivity of the calculations. The reduction in rate constant was accomplished by increasing the activation energy although arguments could be made for decreasing the preexponential. It was felt that, since the reaction is spin-hindered, a higher activation energy might be required to achieve an excited transition state from which the reaction could be completed.



For the case of normal combustion between 80 and 125 per cent stoichiometric air there would be very little difference whether the activation energy or the preexponential were adjusted to reduce the rate constant. Within that range of stoichiometries the temperature variation causes only a factor of two variation in the rate constant even for the higher activation energy. A more significant difference would be noted for modified combustion where the temperature differences would be greater.

** The initially estimated rate coefficient of $2 \times 10^{13} e^{-(13,000/RT)}$ was based on an original estimate by Benson, Golden and Shaw of SRI (private communication). Their estimate was subsequently revised to $1 \times 10^{11} e^{(-19,000/RT)}$ as reported in EPA-600/2-75-019.

The initially estimated rate constant used for the $CH + N_2$ reaction, $2 \times 10^{13}\ e^{-(13{,}000/RT)}$, resulted in a prediction of 4000 ppm of NO_x at 2 msec residence time. With the base rate reduced by one order of magnitude (by increasing the activation energy by 10 kcal) the NO_x level dropped to 2000 ppm. Reducing the base rate by two orders of magnitude, dropped the NO_x level to 300 ppm, and reducing the rate by another order of magnitude dropped the NO_x level to 50 ppm. Another half order of magnitude lower on the rate constant resulted in a prediction of 39 ppm at 2 msec. Based on comparison of these calculations with experimental results for the adiabatic stirred combustor, the rate expression $k = 2 \times 10^{13}\ e^{-(48{,}000/RT)}$ was found to give the best agreement (see Sections 3.3 and 3.4 for further detail).

Another interesting observation was that the predicted NO_x concentration at 80 per cent stoichiometric air was higher than that at 100 per cent stoichiometric air for all cases except the lowest $CH + N_2$ rate used. This observation is consistent with the fact that peak NO_x formation in the jet-stirred combustor occurs experimentally between 85 and 90 per cent stoichiometric air. The variation in predicted NO_x concentration with activation energy of the $CH + N_2$ reaction is shown in Figure 3-4. The importance of various reactions and the comparison with Adiabatic Stirred Combustor data will be discussed in subsequent sections.

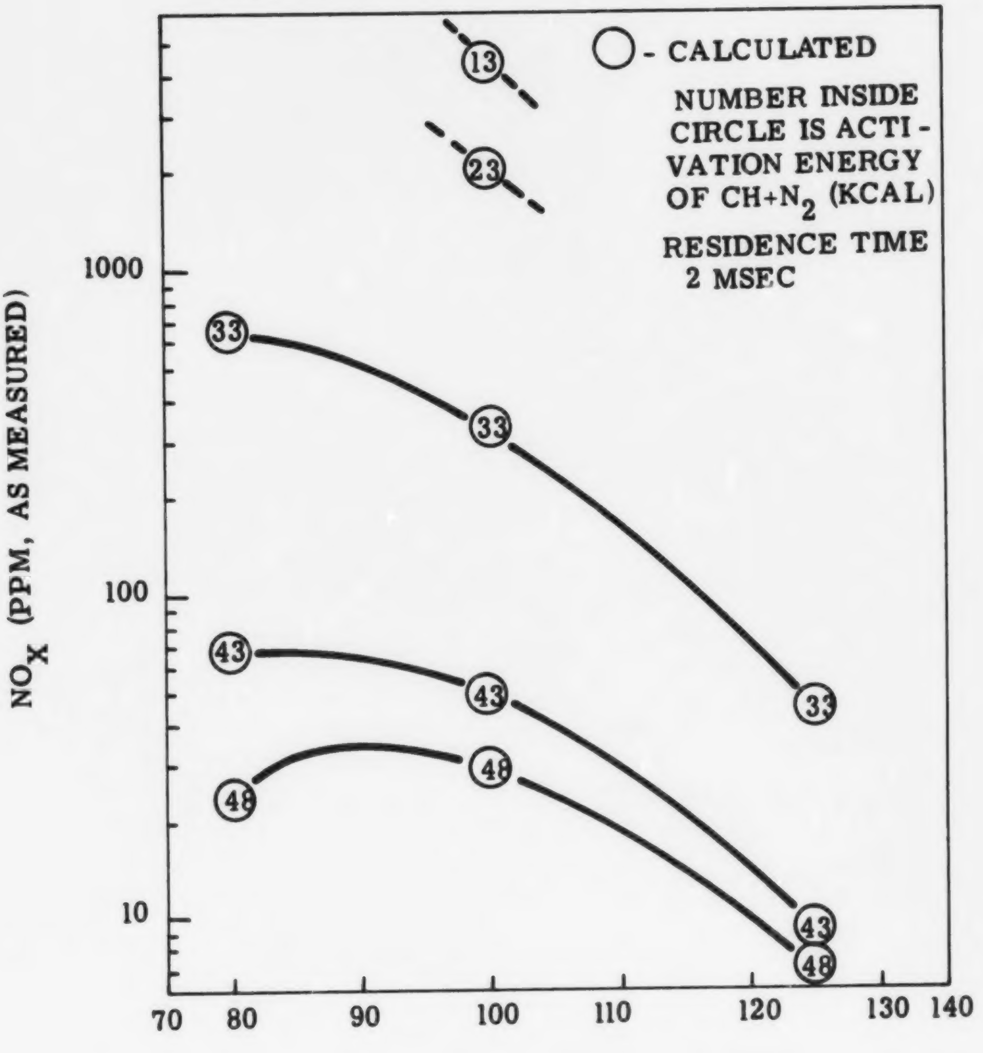
The same set of rate constants was used to predict stirred reactor performance under modified combustion conditions. Combustion modification conditions studied were preheat, water addition and flue gas recirculation. To provide cross-comparisons between calculations, 473°K preheat was used for all modified combustion.

For the case of 473°K preheat in methane/air combustion in a stirred reactor the NO_x level predicted was 75 ppm at 2 msec residence time compared to 29 ppm predicted for no preheat. Predicted temperature was 2155 K compared to 2049 for no preheat. Thus, the increase of approximately 100°K in combustion temperature resulted in the NO_x level somewhat more than doubling. This indicates an overall activation energy of 61 kcal over that range of temperature.

For the case of 2% (on air) water addition (equivalent to about 25% on fuel) with 473°K preheat the calculated temperature was 2128 K compared to 2155 K with no water and 2049 K with no water and no preheat. Prevaporized water was used in the calculations since 473 K preheat was used. If liquid water had been used, the heat of vaporization would have further depressed the temperature. The NO_x level calculated for 2% water addition was 53 ppm, a 30% drop from the 75 ppm without water addition. At the 5% level of water addition, the temperature dropped to 2088 K with a corresponding drop in NO_x to 36 ppm, better than 50% below the results for no water addition. Since the results apparently show no effect other than those expected from the concentration and temperature effects, it is concluded that water addition under these conditions has primarily a thermal effect. While there were small effects in the concentrations of the important intermediates, no major changes in mechanism were noted for the case of water addition. The concentration of water in the stirred reactor increased from 17%, in the case of no water addition, to 20%, in the case of 5% water addition.

FIGURE 3-4

ADIABATIC STIRRED COMBUSTOR METHANE AIR



Flue gas recirculation also had a strong thermal effect. At the level of 10% recirculation (10% of the exhaust gas recirculated--note that at 50% FGR, the recirculated gas is equal to the fresh reactants to the burner) the temperature dropped from 2155 K to 1928 K and the NO_x dropped to 9 ppm. At 25% recirculation, the temperature calculated was 1739 K and the NO_x was calculated to be 1 ppm. At 50% recirculation the temperature dropped to 1387 K and the calculated NO_x was substantially less than 1 ppm. At the higher levels of flue gas recirculation, although only low levels of NO_x were formed, the Zeldovich mechanism became dominant and the $CH + N_2$ reaction played only a minor role. Even though the $N_2 + O$ reaction has a higher activation energy, the CH concentration dropped off to make the $CH + N_2$ reaction even slower. No additional mechanism was found to come into play at lower temperatures in these calculations.

3.2.2 Hydrogen/Air Combustion

Calculations for hydrogen-air combustion were carried out with the subset of the methane/air reactions that involved only H- O- or N-containing species. Adjustments to the rates were not made during the calculations. The predictions for NO_x levels for hydrogen/air combustion are shown in Figure 3-5.

3.2.3 Carbon Monoxide-Air Combustion

Calculations for carbon monoxide/air combustion were carried out by adding the CO and CO_2 reactions to the hydrogen/air combustion reaction set. Calculations were performed for both "wet" and "dry" CO cases. The molar ratios of hydrogen to CO in these cases were 0, 0.01 and 0.10.

It was found that dry CO calculations ($H_2/CO = 0$) resulted in blowout at all mixture ratios but that ratios of 0.01 and 0.10 resulted in stable calculations. No search was made for the minimum stable H_2/CO ratio.

The calculations for 1% H_2 and 10% H_2 in CO are illustrated in Figure 3-6. Peak NO_x concentrations appear to occur at about 90 per cent stoichiometric air in both cases.

3.3 Reactions of Importance for Methane/Air Combustion

The calculations for methane/air combustion and pollutant formation in a stirred reactor were accomplished using the pre-screened set of 101 reactions indicated previously. These reactions were used over the range of 80-125% stoichiometric air and while there were mechanistic differences among fuel-rich, stoichiometric, and fuel-lean combustion, these differences were more in matters of degree rather than total changes. The reactions found to be of importance for the stirred reactor calculations performed should find application to the combustion zone of conventional flames. These calculations are not intended to be applicable to the ignition (or branching) zone and the post-flame zone. The results of any kinetics calculation are, of course, dependent on the particular set of rate constants used in the calculations but the comments in this section are intended to highlight findings of general applicability.

FIGURE 3-5

CALCULATED NO_X LEVELS IN H_2-AIR COMBUSTION

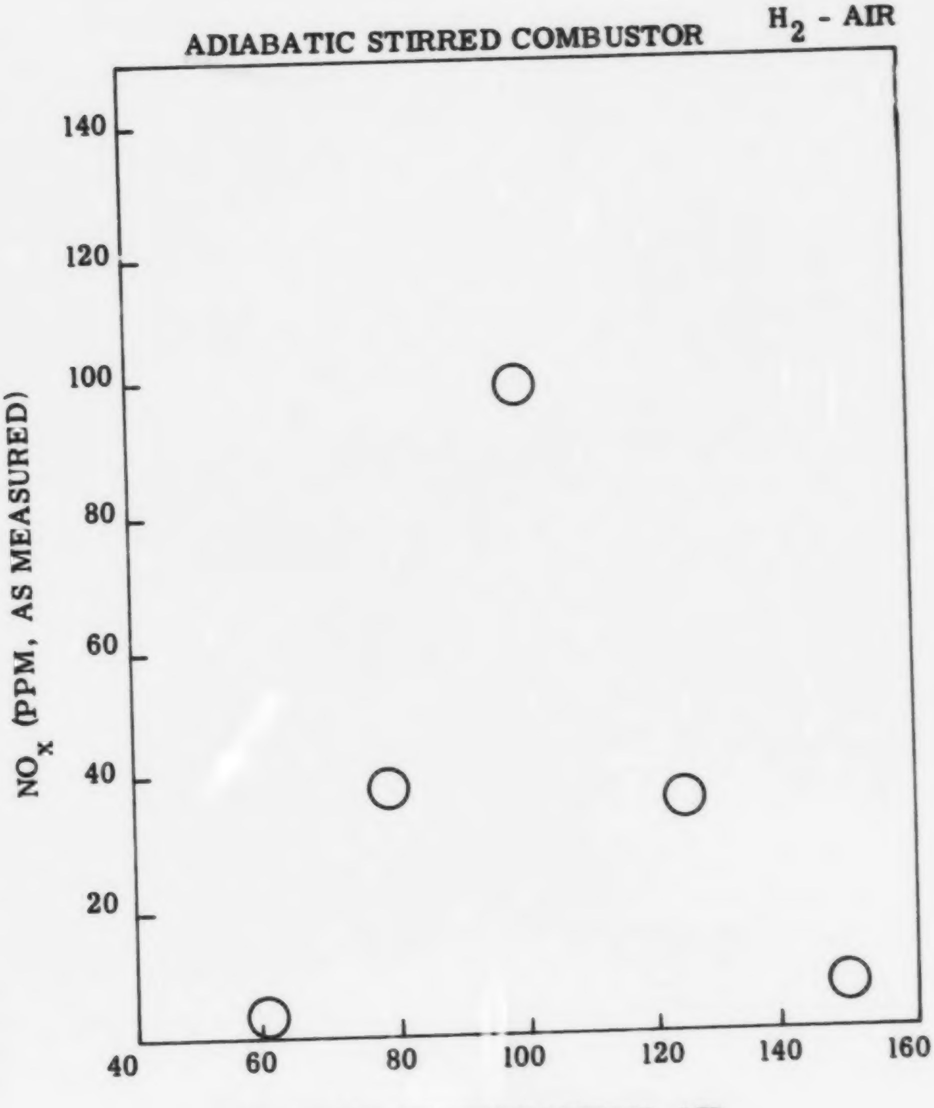
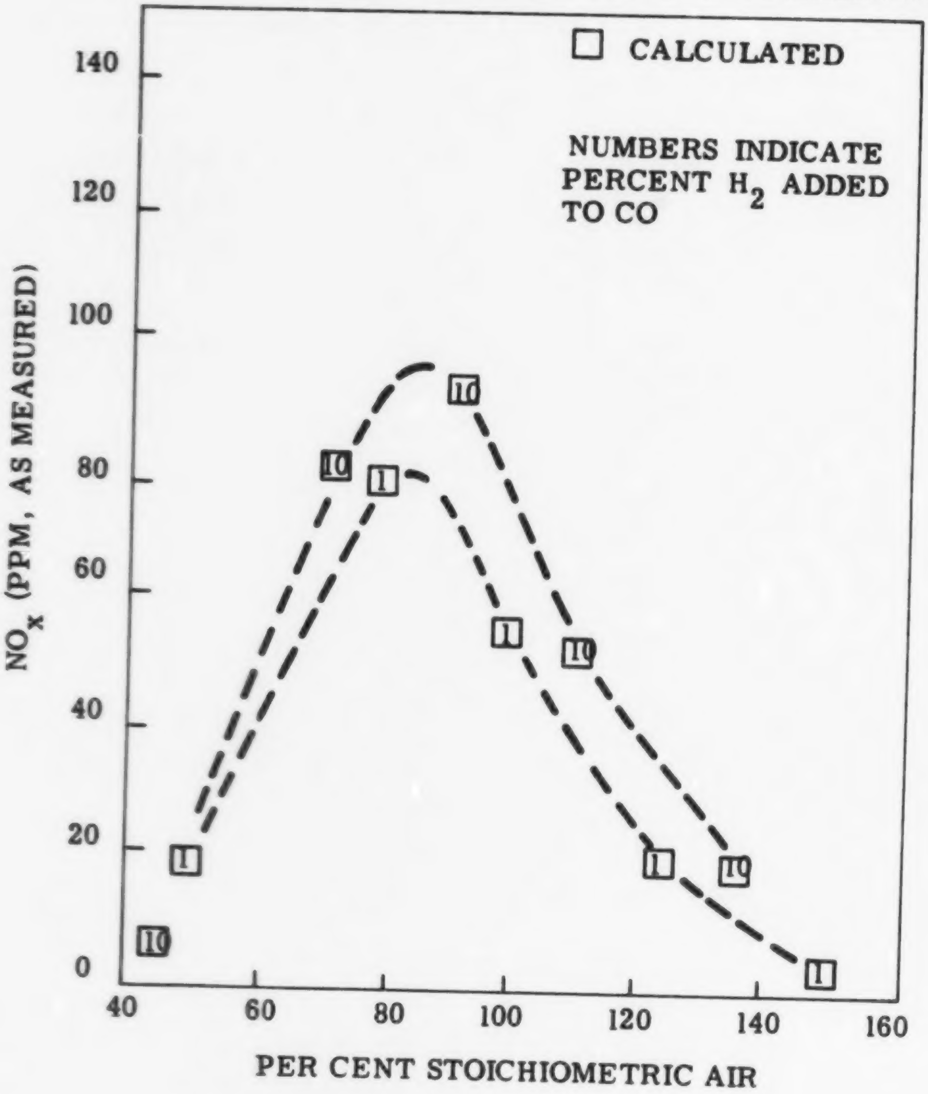


FIGURE 3-6

ADIABATIC STIRRED COMBUSTOR CARBON MONOXIDE-AIR



The overall mechanism for methane combustion between 80 and 125% stoichiometric air proceeds primarily through the intermediates CH_3, CH_2O, CHO, CO and finally to CO_2. That portion of the CH_3 that finds its way to CH_3O is returned through CH_2O. Small portions of the CH_3 proceed through CH_2 and CH but essentially all of these intermediates return through CH_2O, CHO and CO. The reaction path is indicated schematically in Figure 3-7a,b,c for 80%, 100% and 125% stoichiometric air. The numbers indicate the percentage of each intermediate proceeding to the next intermediate, by one or more of the reactions considered. This figure is intended to illustrate the gross path of the combustion intermediates between CH_4 and CO_2. The numbers have been rounded for the purpose of this illustration. A more complete discussion of the reactions and their relative importance will be presented later in this section. A schematic of the combustion reactions and their connection with NO_x-forming reactions is shown in Appendix C. The major feature to be noted in Figure 3-7 is the similarity between the reaction paths for the main intermediates for the three stoichiometries. The main differences occur in the manner in which CH_2 and CH are returned to the main reaction path at the different stoichiometries.

While the main combustion path shows relatively minor differences at the different stoichiometries, somewhat larger differences are noted in the reactions of importance for NO_x formation. These reactions which are so important for NO_x are relatively unimportant for the gross combustion mechanism. A species schematic for NO_x formation is shown in Figure 3-8. The figures at the tails of the arrows indicate the percentage of each intermediate proceeding to the next intermediate, by one or more of the reactions considered, and the figures at the heads of the arrows indicate the percentage of each intermediate formed by reaction of the preceding intermediates. The numbers have been rounded for the purpose of this illustration.

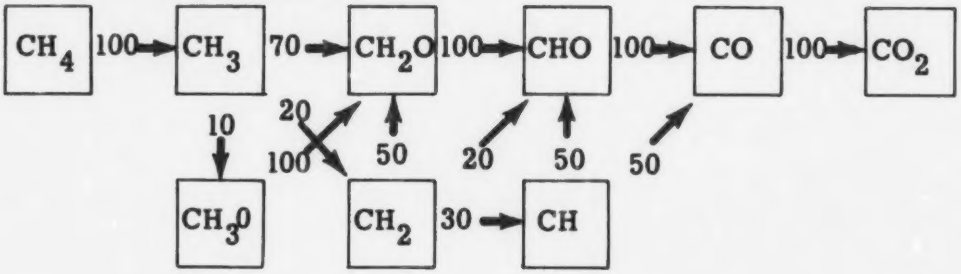
It is interesting to note that all of the N atoms proceed to form NO and that N atoms are formed primarily by the breaking of the N_2 molecule by oxygen atom or by hydrocarbon radicals. Essentially all of the NO is formed from N_2 molecules and N atoms with N_2O beginning to play a role under fuel-lean conditions. For the stirred reactor, any NO_2 that is formed appears to recycle back to NO almost quantitatively.

To examine in more detail specific reactions involved in methane combustion and pollutant formation in a stirred reactor, consider the results for the set of 101 prescreened reactions discussed earlier. Table 3-3 contains information on the production and destruction of selected species by the reactions found to have the major effects on those species in the kinetics calculations. The numbers in Table 3-3 refer to the results for the specific rate constants used in these calculations and are provided for illustration of those results. While further refinement of the rate constants may result in changing these numbers, it is expected that the major conclusions that can be drawn from these calculations would not be negated by such refinements. For example, the precise percentage of CH_4 that reacts by way of $CH_4 + OH \rightarrow CH_3 + H_2O$ may be changed by refinements in rate constants but the fact that $CH_4 + OH \rightarrow CH_3 + H_2O$ plays a major role in CH_4 breakdown is not expected to be changed by such refinements.

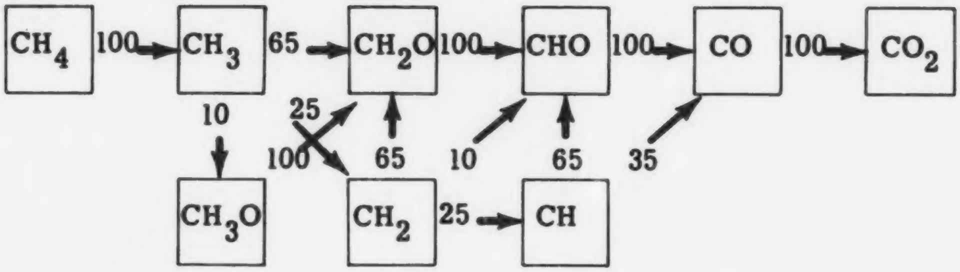
FIGURE 3-7

PATHS FOR COMBUSTION INTERMEDIATES BETWEEN CH_4 AND CO_2

A. 80% STOICHIOMETRIC AIR


CH4
100
CH3
70
CH2O
100
CHO
100
CO
100
CO2
10
20
100
50
20
50
50
CH3O
CH2
30
CH

B. 100% STOICHIOMETRIC AIR


CH4
100
CH3
65
CH2O
100
CHO
100
CO
100
CO2
10
25
100
65
10
65
35
CH3O
CH2
25
CH

C. 125% STOICHIOMETRIC AIR

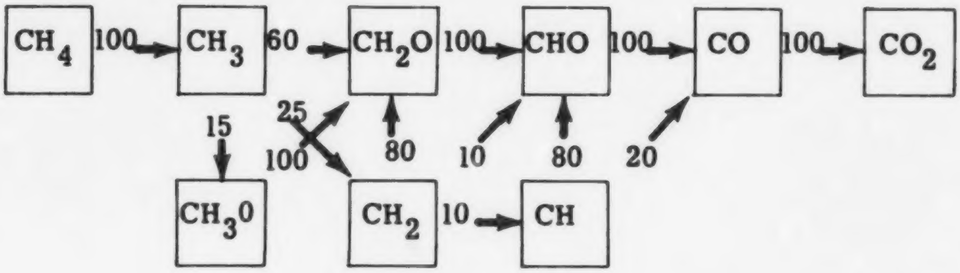

CH4
100
CH3
60
CH2O
100
CHO
100
CO
100
CO2
15
25
100
80
10
80
20
CH3O
CH2
10
CH

FIGURE 3-8a

PATHS FOR INTERMEDIATES INVOLVED IN NO_X FORMATION

A. 80% STOICHIOMETRIC AIR

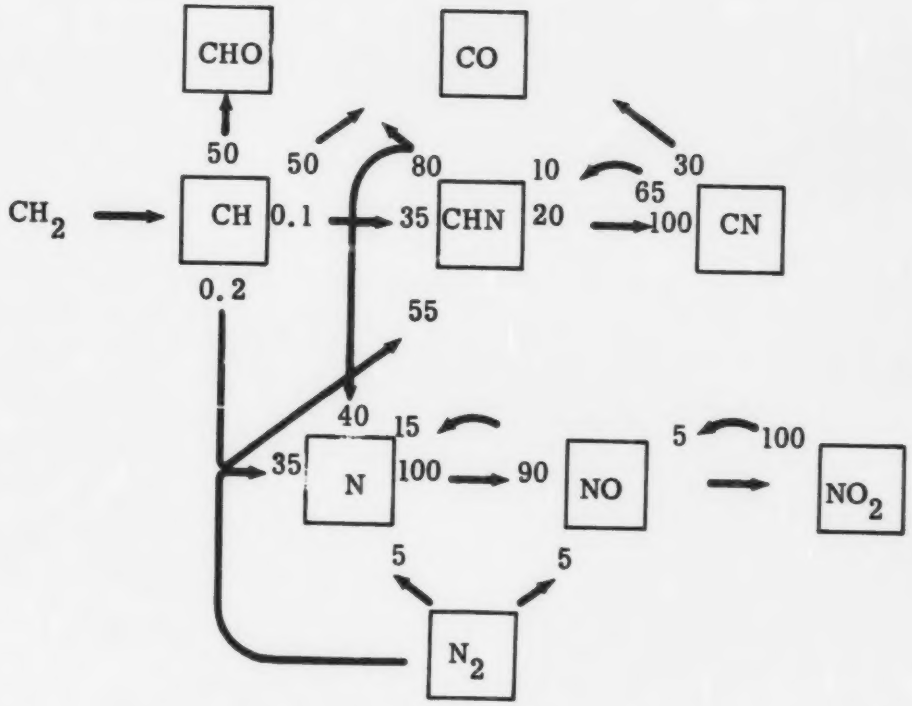

CHO
CO
50
50
80
10
30
65
CH_2
CH
0.1
35
CHN
20
100
CN
0.2
55
40
15
5
100
35
N
100
90
NO
NO_2
5
5
N_2

FIGURE 3-8b

PATHS FOR INTERMEDIATES INVOLVED IN NO_X FORMATION

B. 100% STOICHIOMETRIC AIR

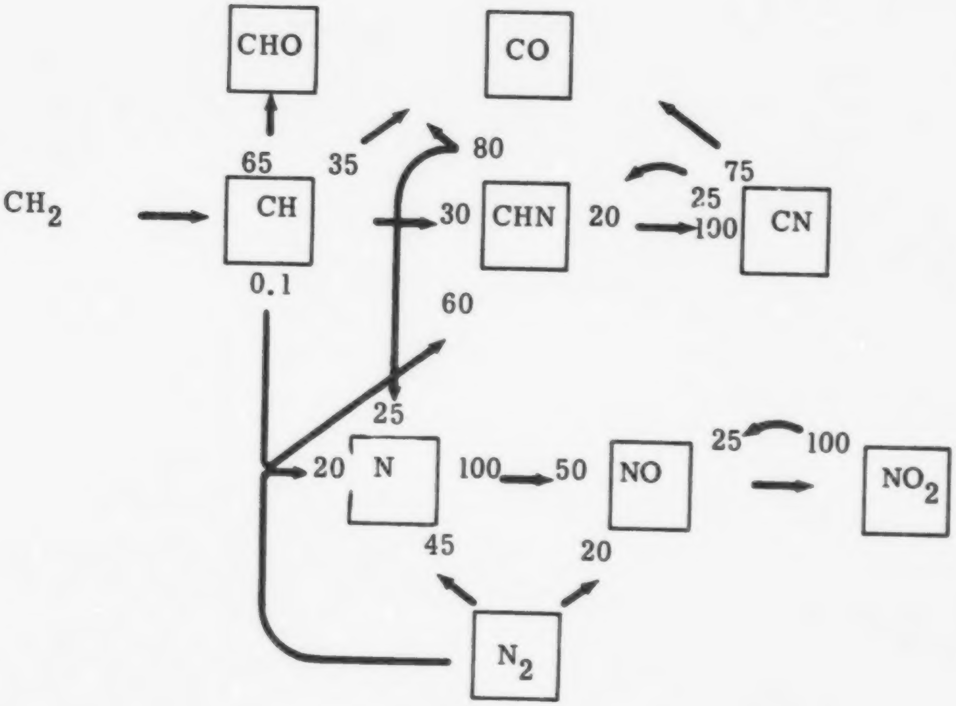

CHO
CO
65
35
80
75
25
CH₂
CH
30
CHN
20
100
CN
0.1
60
25
25
100
20
N
100
50
NO
NO₂
45
20
N₂

FIGURE 3-8c

PATHS FOR INTERMEDIATES INVOLVED IN NO_X FORMATION

C. 125% STOICHIOMETRIC AIR

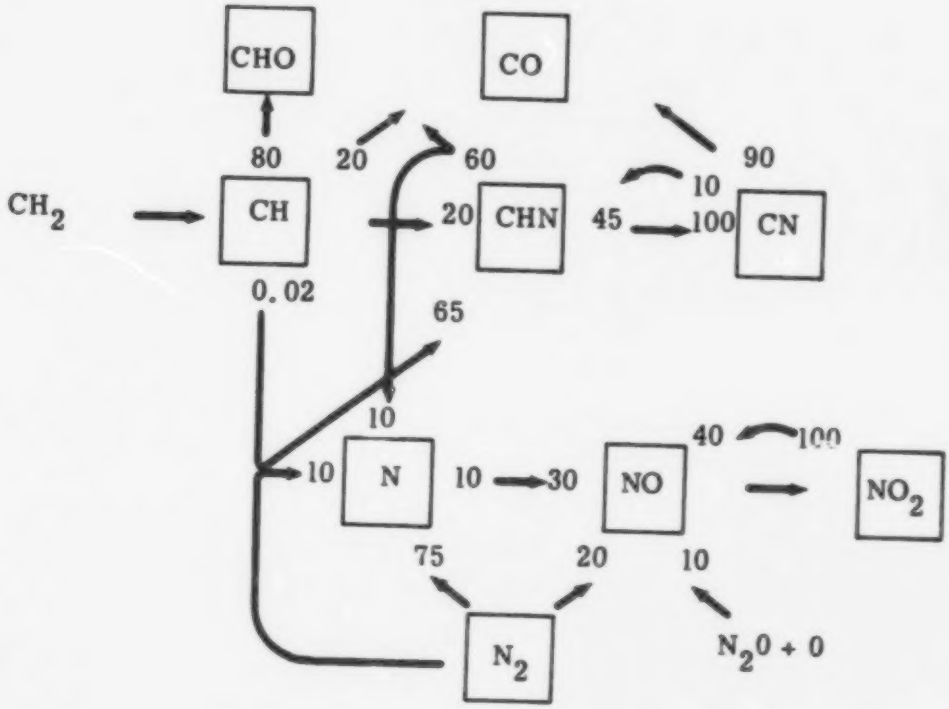

CHO
CO
80
20
60
90
10
CH2
CH
20
CHN
45
100
CN
0.02
65
10
10
N
10
30
NO
40
100
NO2
75
20
10
N2
N2O + O

TABLE 3-3

Production and Destruction of Species by Specific Reactions for Stirred Reactor Calculations

Species	Production Reactions	Per Cent of Production at			Destruction Reactions	Per Cent of Destruction at		
		80	100	125		80	100	125
		Per Cent Stoichiometric Air				Per Cent Stoichiometric Air		
CH_4					$CH_4 + OH \rightarrow CH_3 + H_2O$	56	79	86
					$CH_4 + H \rightarrow CH_3 + H_2$	41	16	7
					$CH_4 + O \rightarrow CH_3 + OH$	3	5	7
CH_3	$CH_4 + OH \rightarrow CH_3 + H_2O$	56	79	86	$CH_3 + O \rightarrow CH_2O + H$	63	60	57
	$CH_4 + H \rightarrow CH_3 + H_2$	41	16	7	$CH_3 + OH \rightarrow CH_2 + H_2O$	12	17	17
	$CH_4 + O \rightarrow CH_3 + OH$	3	5	7	$CH_3 + O \rightarrow CH_2 + OH$	3	7	7
					$CH_3 + H \rightarrow CH_2 + H_2$	2	1	-
					$CH_3 + OH \rightarrow CH_3O + H$	9	11	13
					$CH_3 + H + M \rightarrow CH_4 + M$	10	2	1
CH_3O	$CH_3 + OH \rightarrow CH_3O + H$	100	100	100	$CH_3O + M \rightarrow CH_2O + H + M$	96	97	98
CH_2O	$CH_3 + O \rightarrow CH_2O + H$	76	67	61	$CH_2O + OH \rightarrow CHO + H_2O$	62	68	67
	$CH_3O + M \rightarrow CH_2O + H + M$	11	12	13	$CH_2O + O \rightarrow CHO + OH$	15	25	30
	$CH_2 + O_2 \rightarrow CH_2O + O$	4	14	20	$CH_2O + H \rightarrow CHO + H_2$	23	7	3
	$CH_2 + OH \rightarrow CH_2O + H$	7	4	2				

TABLE 3-3 (Continued)

Species	Production Reactions	Per Cent of Production at Per Cent Stoichiometric Air			Destruction Reactions	Per Cent of Destruction at Per Cent Stoichiometric Air		
		80	100	125		80	100	125
CH_2	$CH_3 + OH \rightarrow CH_2 + H_2O$	68	70	70	$CH_2 + O_2 \rightarrow CH_2O + O$	20	49	75
	$CH_3 + O \rightarrow CH_2 + OH$	17	22	28	$CH_2 + OH \rightarrow CH_2O + H$	31	16	7
	$CH_3 + H \rightarrow CH_2 + H_2$	14	4	2	$CH_2 + O \rightarrow CHO + H$	16	12	7
					$CH_2 + OH \rightarrow CH + H_2O$	32	23	11
CH	$CH_2 + OH \rightarrow CH + H_2O$	97	99	100	$CH + O_2 \rightarrow CHO + O$	24	55	78
					$CH + OH \rightarrow CHO + H$	18	9	3
					$CH + O \rightarrow CO + H$	40	29	18
CHO	$CH_2O + OH \rightarrow CHO + H_2O$	57	63	64	$CHO + M \rightarrow CO + H + M$	92	93	94
	$CH_2O + O \rightarrow CHO + OH$	14	23	29				
	$CH_2O + H \rightarrow CHO + H_2$	21	6	3				
	$CH_2 + O \rightarrow CHO + H$	3	3	2				
	$CH + O_2 \rightarrow CHO + O$	2	3	2				
	$CH + OH \rightarrow CHO + H$	1	1	-				
CO	$CHO + M \rightarrow CO + H + M$	89	91	93	$CO + OH \rightarrow CO_2 + H$	89	93	95
					$CO + O + M \rightarrow CO_2 + M$	11	7	5

TABLE 3-3 (Continued)

Species	Production Reactions	Per Cent of Production at 80	100	125	Destruction Reactions	Per Cent of Destruction at 80	100	125
		Per Cent Stoichiometric Air				Per Cent Stoichiometric Air		
CO_2	$CO + OH \rightarrow CO_2 + H$	89	93	95				
	$CO + O + M \rightarrow CO_2 + M$	11	7	5				
HCN	$CH + N_2 \rightarrow HCN + N$	52	58	64	$HCN + O \rightarrow CHO + N$	81	81	57
	$CH + NO \rightarrow HCN + O$	36	31	21	$HCN + OH \rightarrow CN + H_2O$	18	19	43
	$CH_4 + CN \rightarrow HCN + CH_3$	8	4	4				
	$CH_2 + N_2 \rightarrow HCN + NH$	3	6	10				
CN	$HCN + OH \rightarrow CN + H_2O$	97	99	99	$CN + CH_4 \rightarrow CH_3 + HCN$	63	24	12
					$CN + O_2 \rightarrow CO + NO$	12	52	76
					$CN + O \rightarrow CO + N$	15	21	10
N	$CH + N_2 \rightarrow HCN + N$	33	19	11	$N + OH \rightarrow NO + H$	96	83	59
	$HCN + O \rightarrow CHO + N$	36	23	8	$N + O_2 \rightarrow NO + O$	4	17	41
	$N_2 + O \rightarrow NO + N$	5	42	73				
	$CH + NO \rightarrow CHO + N$	14	7	2				
	$CH_2 + NO \rightarrow CH_2O + N$	9	7	5				

TABLE 3-3 (Continued)

Species	Production Reactions	Per Cent of Production at 80 Per Cent Stoichiometric Air	100	125	Destruction Reactions	Per Cent of Destruction at 80 Per Cent Stoichiometric Air	100	125
NO	$N + OH \rightarrow NO + H$	83	40	16	$NO + CH \rightarrow HCN + O$	42	14	-
	$N + O_2 \rightarrow NO + O$	4	9	11	$NO + CH \rightarrow CHO + N$	25	9	-
	$N_2 + O \rightarrow NO + N$	5	21	20	$NO + HO_2 \rightarrow NO_2 + OH$	7	51	85
	$NO_2 + H \rightarrow NO + OH$	5	23	37	$NO + O + M \rightarrow NO_2 + M$	4	13	15
	$N_2O + O \rightarrow NO + NO$	-	2	11	$NO + CH_2 \rightarrow CH_2O + N$	18	9	-
NO_2	$NO + HO_2 \rightarrow NO_2 + OH$	61	79	85	$NO_2 + H \rightarrow NO + OH$	100	98	95
	$NO + O + M \rightarrow NO_2 + M$	39	21	15				

The numbers shown in Table 3-3 represent the relative contribution of a given reaction to the sum of all of the reactions that produce or destroy a given species. The numbers do not represent the absolute level of production or destruction. In fact the major "production" of CH_4, N_2, and O_2 occurs from the input of these species as reactants. If there were entries for production of CH_4 in the table, the major reaction for production of CH_4 would be insignificant compared to the reactant input. As another example it will be noted that at 125% stoichiometric air the only destruction reactions for NO result in the formation of NO_2. It should be noted, however, that very little of the NO is destroyed in this manner relative to the NO output from the reactor and most of the NO_2 so formed is destroyed by a reaction that produces NO.

Since the main path for the combustion reactions involves $CH_4 \rightarrow CH_3 \rightarrow CH_2O \rightarrow CHO \rightarrow CO \rightarrow CO_2$, the production and destruction reactions for these species are readily ascertained by inspection of Table 3-3. The production and destruction of some of the minor species is not so straightforward and will be discussed in more detail here.

The species of prime interest for this study is NO and therefore attention will be focused on NO and its precursors. Working backwards from NO, the following observations are noted:

- NO production is dominated under fuel rich and stoichiometric air conditions by reactions of N atoms with N + OH more important than $N + O_2$.
- NO production from $N_2 + O$ is relatively unimportant under fuel rich and relatively important under fuel lean conditions
- Production of NO from NO_2 results from the loop $NO \rightarrow NO_2 \rightarrow NO$.
- Production of NO from N_2O begins to become significant under fuel lean conditions but is not dominant at 125% stoichiometric air.

Going back one step to N atom, the following observations are noted:

- Under fuel rich conditions N is produced primarily by $CH + N_2 \rightarrow HCN + N$.
- Most of the HCN produced by $CH + N_2 \rightarrow HCN + N$ also ends up as N.
- Under stoichiometric air conditions the N from $CH + N_2$ and from HCN is comparable to that from $N_2 + O$.
- Under fuel lean conditions N is formed primarily from $N_2 + O \rightarrow NO + N$.

Examining the reactions of importance for CH it is found that:

- While $CH + N_2 \rightarrow HCN + N$ is important for N atom production and HCN production, it does not play a major role in CH destruction (less than 1%).
- CH is produced primarily by $CH_2 + OH \rightarrow CH + H_2O$.
- CH is destroyed by reactions with O, OH and O_2.

Since CH is produced almost exclusively from CH_2, inspection of the CH_2 reactions indicates:

- Between 10 and 30% of the CH_2 winds up as CH through the reaction $CH_2 + OH \rightarrow CH + H_2O$.
- CH_2 is produced almost exclusively from CH_3 by reactions with OH, O and H.
- Between 15 and 25% of the CH winds up as CH_2.
- CH_3 is produced from CH_4 and CH_4 goes primarily to CH_3.

Regarding HCN

- HCN is produced primarily by $CH + N_2 \rightarrow HCN + N$ and secondarily from $CH + NO \rightarrow CHN + O$.
- HCN ultimately yields N or CN in the present calculations.
- The CN, resulting primarily from HCN, yields NO or HCN or N atom which ultimately result in NO.

Thus, from the above observations the key reactions that should receive further study are first, the most obvious

$$CH + N_2 \rightarrow HCN + N$$

and second, the reactions that produce CH such as

$$CH_2 + OH \rightarrow CH + H_2O$$

and that produce CH_2 such as

$$CH_3 + OH \rightarrow CH_2 + H_2O$$

It might in fact be easier to study the reverse of the last two reactions even though the forward rate is of primary interest. Measurements of N atom concentrations as well as CH and CH_2 concentrations in a stirred reactor would provide valuable insight into the kinetics and mechanism of NO formation in flames.

Thus, hydrocarbon species appear to play a major role in NO_x formation in the flame zone under specific conditions. This would imply that under conditions where NO_x in the flame zone could be important (i.e. when one is trying to reduce NO_x emissions below 100 ppm) the CH concentration could play a major role.

3.4 Comparison of Theoretical Calculations with Experimental Results

The kinetics calculations for hydrogen/air, carbon monoxide/air and methane/air combustion under normal firing conditions were compared with experimental results reported in Section 2. Those comparisons are reported in this section.

The experimental results for hydrogen/air combustion were limited to temperatures below 2200 K and therefore only limited data were taken in the adiabatic stirred combustor. However, where data were available the agreement with calculations was good as shown in Figure 3-9.

The experimental results for carbon monoxide/air were restricted to the same upper temperature limit as the hydrogen data. Experiments were conducted with hydrogen addition ranging from 0-17% of the carbon monoxide. Calculations were performed for 0, 1, and 10% hydrogen addition. While the 1% and 10% additions yielded stable solutions, the 0% calculation indicated blowout. No attempt was made to dry the air in the experimental system and the moisture content of the air used is uncertain although reasonably dry. The experimental results are compared with the calculations in Figure 3-10 and show reasonably good agreement.

The methane/air experiments were run over the range 85-130% stoichiometric air at a residence time of 2.5 milliseconds. Most of the calculations were performed at 2 milliseconds with variations to 3 and 5 milliseconds. The plot and the shape of the curve shown in Figure 3-11 are based on the parametric variation of the $CH + N_2$ reaction rate and comparison with previously obtained stirred reactor data as discussed in Section 3.2. The final rate used for the $CH + N_2$ reaction* was $k_f = 2 \times 10^{13} e^{-(48{,}000/RT)}$. This matching procedure is also in good agreement with extensive stirred reactor data on methane/air taken previously on a non-adiabatic system.

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* The final rate was 3.5 orders of magnitude lower than the base case estimate.. All of the adjustment was made in the activation energy as discussed previously. However, while the experimental data definitely indicated that the rate had to be slower than the original estimate, it could not be determined unequivocally whether the preexponential should be lower or the activation energy should be higher.

FIGURE 3-9

ADIABATIC STIRRED COMBUSTOR HYDROGEN-AIR

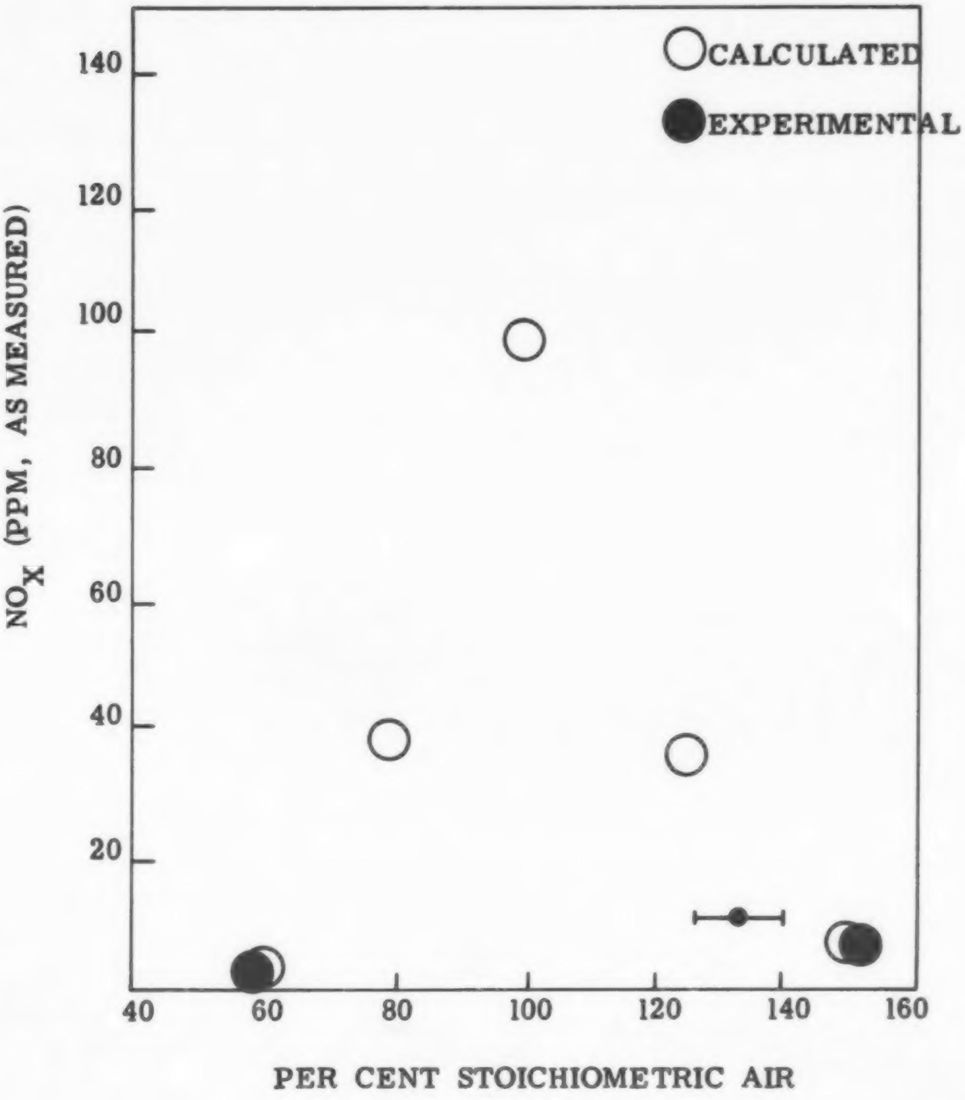


FIGURE 3-10

ADIABATIC STIRRED COMBUSTOR CARBON MONOXIDE-AIR

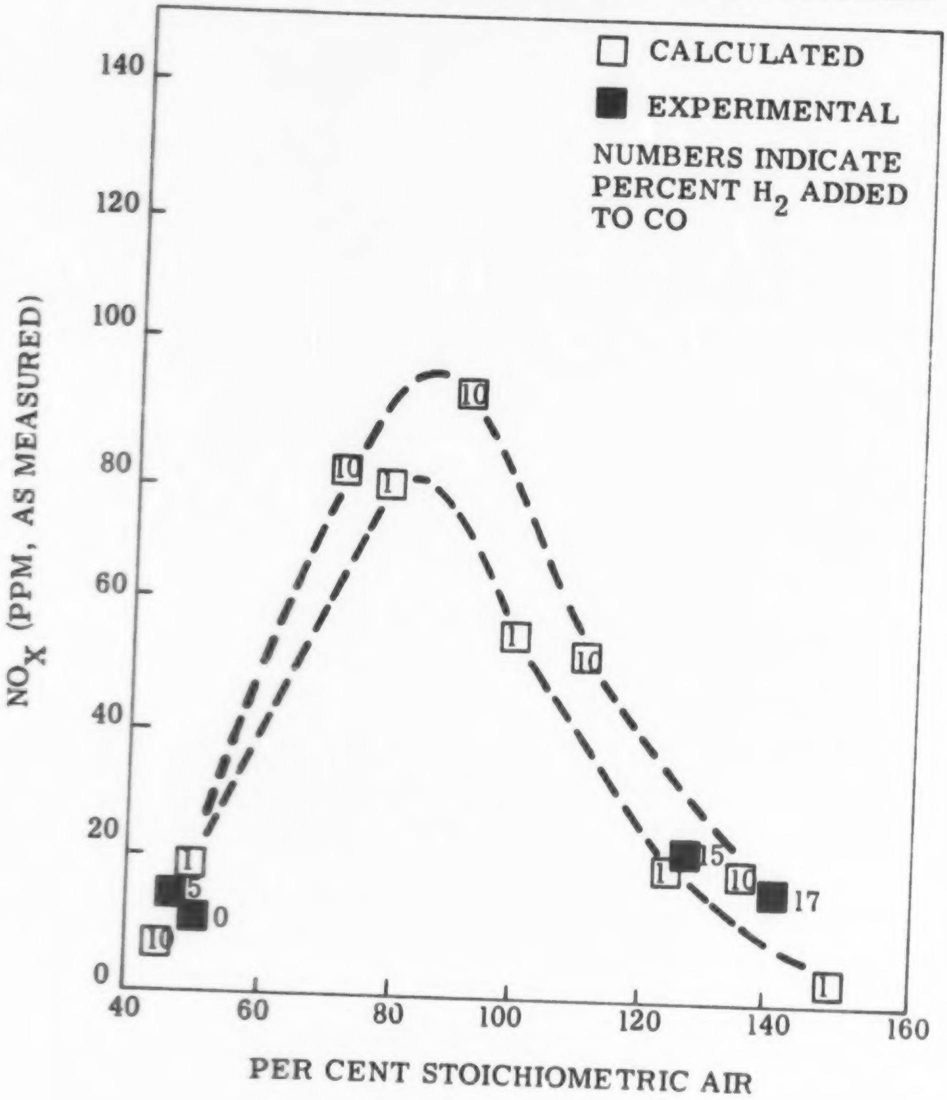
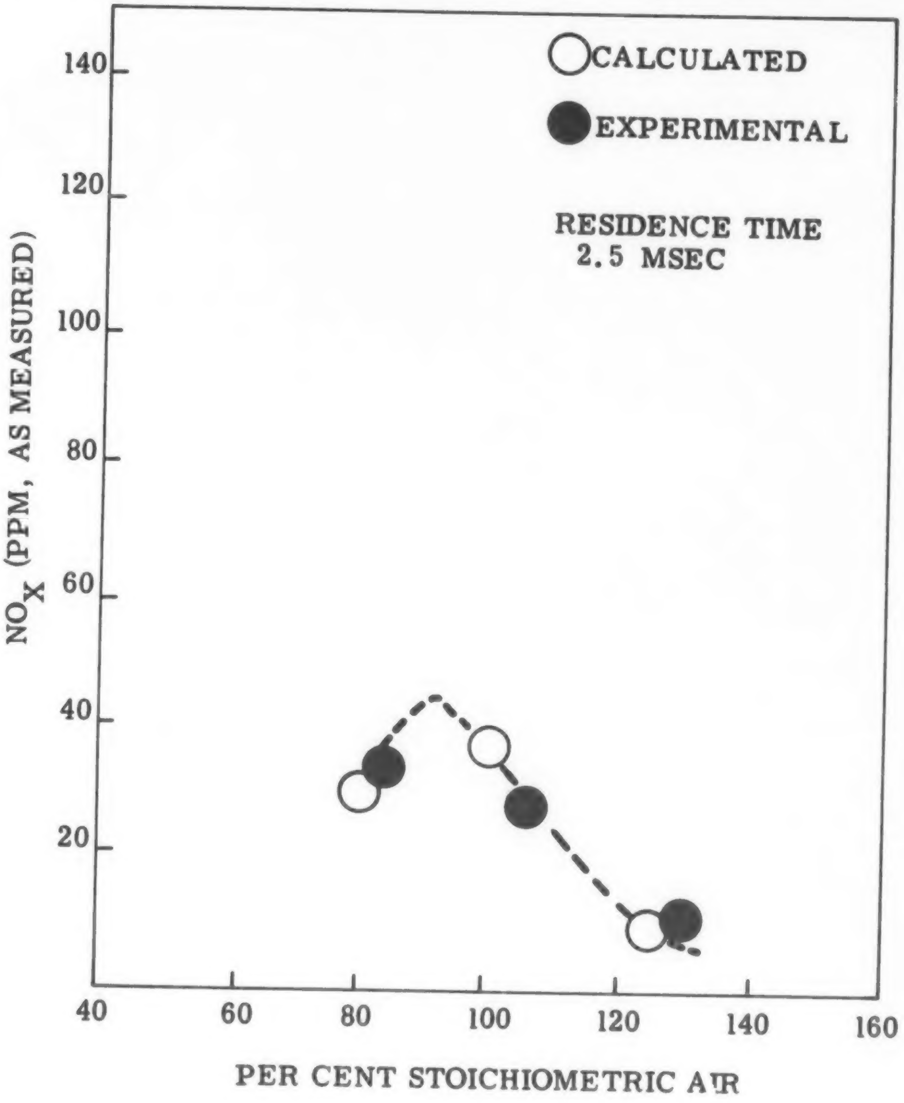


FIGURE 3-11

ADIABATIC STIRRED COMBUSTOR METHANE AIR



4. CONCLUSIONS AND RECOMMENDATIONS

1. The Adiabatic Stirred Combustor has been shown to be a useful tool for the study of the chemistry of combustion coupled to pollutant formation

   - The stirred zone was shown to be well-stirred, matching the results of the jet-stirred combustor with hemispherical geometry under comparable conditions.

   - The radial profiles at the exit of the stirred zone were shown to be flat and continued to be flat downstream of the stirred zone.

2. The approach to kinetics calculations of combustion by starting from a reaction set containing all possible unimolecular and bimolecular reactions was shown to be valuable for the investigation of methane/air combustion. This approach allows investigation of competitive mechanisms that might otherwise be overlooked by an intuitive approach to such a complex system. It should be noted, however, that the success of such an approach is also dependent on the accuracy with which the individual rate constants are known. In addition, the magnitude of the task increases exponentially with the number of species considered. This fact makes the analysis of the combustion of higher hydrocarbons more difficult using this technique.

3. The calculations for hydrogen and carbon monoxide combustion in the adiabatic stirred combustor match the data quite well.

4. The formation of NO during combustion of methane/air in the adiabatic stirred combustor is also matched well and the results lead to some interesting conclusions:

   (a) The formation of NO_x is controlled by the concentrations of both N atoms and O atoms.

   (b) Under fuel lean conditions the concentration of N atoms is controlled by the concentration of O atoms through the reaction $N_2 + O \rightarrow NO + N$.

   (c) Under fuel rich conditions, however, the concentration of N atoms is controlled by the reaction $CH + N_2 \rightarrow HCN + N$ and the production of NO is predominantly through N atoms by way of $N + OH \rightarrow NO + H$. The HCN produced eventually results in the formation of more N atoms.

   (d) Under stoichiometric air conditions, the production of N atoms is balanced between $N_2 + O \rightarrow N + O_2$ and $CH + N_2 \rightarrow HCN + N$.

5. The results of these calculations indicate that further study is warranted on the reaction $CH + N_2 \rightarrow HCN + N$. Studies are also warranted on the reactions that lead to CH formation such as $CH_2 + OH \rightarrow CH + H_2O$ and $CH_3 + OH \rightarrow CH_2 + H_2O$. Reactions of HCN that lead to the formation of N atom should also be studied.

6. Measurements of the concentrations of species such as N, CH, and CH_2 during hydrocarbon combustion are required for the further elucidation of the mechanism of NO_x formation.

7. Calculations on combustion modification experiments in the stirred reactor indicate that further information on the key reactions in NO_x formation could be obtained from such experiments. The activation energy of the $CH + N_2$ reactions could be investigated by flue gas recirculation experiments with either real or simulated flue gases.

8. New calculation techniques should be developed to determine the sensitivity of a given mechanism to each of the component steps. Such techniques would be valuable for application to complex combustion mechanisms such as studied in this investigation. This would allow a determination of the most crucial reactions and the sensitivity of the result to these reactions without individual or multiple repetitive rate adjustments.

9. As new information on the individual reaction rates becomes available, this information should be factored into the set of recommended rates. This is especially important for the key reactions in the mechanism.

10. Understanding of the coupling of the combustion mechanism with NO_x formation becomes increasingly important as the target NO_x levels become lower. An understanding of the involvement of hydrocarbon radicals in the NO formation mechanism through reactions such as $CH + N_2 = CHN + N$ is important both under conventional combustion as well as under modified combustion conditions. Under conditions where this reaction plays a major role, the N atom concentration becomes more important than the O atom concentration in determining NO_x levels. In fact only very low concentrations of CH can result in major changes in NO.

APPENDIX A
DATA LISTINGS

RUN NUMBER 333
PREMIXED FLAT FLAME BURNER
STAGED COMBUSTION
METHANE COLD WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STOIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.076	0.866	119.6	0.000	119.6	32.50	0.00		16	17	3.50	0.000	8.14	0.
0.082	0.866	110.3	0.000	110.3	32.50	0.00		29	31	2.70	0.000	8.87	0.
0.088	0.866	102.2	0.000	102.2	32.50	0.00		58	60	1.60	0.000	9.60	0.
0.095	0.866	95.1	0.000	95.1	32.50	0.00		88	90	0.14	0.000	10.98	0.
0.102	0.866	88.8	0.000	88.8	32.50	0.00		68	69	0.09	1.240	9.92	0.
0.076	0.866	119.6	0.219	149.9	32.50	0.00		11	12	6.20	0.000	6.59	0.
0.082	0.866	110.3	0.219	138.3	32.50	0.00		26	27	5.10	0.000	7.21	0.
0.088	0.866	102.2	0.219	128.1	32.50	0.00		47	48	4.30	0.000	7.83	0.
0.095	0.866	95.1	0.219	119.2	32.50	0.00		68	69	3.30	0.000	8.66	0.
0.102	0.866	88.8	0.219	111.3	32.50	0.00		38	45	3.10	1.182	7.93	0.
0.076	0.866	119.6	0.291	159.9	32.50	0.00		11	12	6.60	0.000	6.18	0.
0.082	0.866	110.3	0.291	147.5	32.50	0.00		23	24	5.90	0.000	6.69	0.
0.088	0.866	102.2	0.291	136.7	32.50	0.00		50	51	5.00	0.000	7.42	0.
0.095	0.866	95.1	0.291	127.2	32.50	0.00		70	70	4.00	0.000	8.14	0.
0.102	0.866	88.8	0.291	118.8	32.50	0.00		38	47	3.90	1.269	7.31	0.

RUN NUMBER 334
PREMIXED FLAT FLAME BURNER
STAGED COMBUSTION
METHANE COLD WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STOIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.076	0.866	119.6	0.364	170.0	32.50	0.00		8	9	7.40	0.000	5.66	0.
0.082	0.866	110.3	0.364	156.8	32.50	0.00		20	21	6.60	0.000	6.28	0.
0.088	0.866	102.2	0.364	145.3	32.50	0.00		39	40	5.70	0.000	6.90	0.
0.095	0.866	95.1	0.364	135.2	32.50	0.00		58	58	4.80	0.000	7.52	0.
0.102	0.866	88.8	0.364	126.2	32.50	0.00		30	39	4.60	1.125	7.00	0.
0.076	0.866	119.6	0.438	180.2	32.50	0.00		9	10	7.80	0.000	5.46	0.
0.082	0.866	110.3	0.438	166.2	32.50	0.00		20	21	7.00	0.000	5.87	0.
0.088	0.866	102.2	0.438	154.0	32.50	0.00		37	38	6.30	0.000	6.48	0.
0.095	0.866	95.1	0.438	143.3	32.50	0.00		52	54	5.40	0.000	7.21	0.
0.102	0.866	88.8	0.438	133.8	32.50	0.00		16	33	5.30	0.872	6.69	0.

RUN NUMBER 335
PREMIXED FLAT FLAME BURNER
STAGED COMBUSTION
METHANE COLD WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STOIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.076	0.866	119.6	0.000	119.6	32.50	0.00		22	22	3.50	0.000	8.25	0.
0.082	0.866	110.3	0.000	110.3	32.50	0.00		45	45	2.30	0.000	9.08	0.
0.088	0.866	102.2	0.000	102.2	32.50	0.00		78	79	0.94	0.000	10.49	0.
0.095	0.866	95.1	0.000	95.1	32.50	0.00		73	75	0.09	0.493	10.73	0.
0.102	0.866	88.8	0.000	88.8	32.50	0.00		50	5	0.08	2.506	9.19	0.
0.076	0.866	119.6	0.219	149.9	32.50	0.00		17	17	6.00	0.000	6.90	0.
0.082	0.866	110.3	0.219	138.3	32.50	0.00		33	34	4.90	0.000	7.52	0.
0.088	0.866	102.2	0.219	128.1	32.50	0.00		64	64	3.90	0.000	8.25	0.
0.095	0.866	95.1	0.219	119.2	32.50	0.00		50	51	3.30	0.734	8.14	0.
0.102	0.866	88.8	0.219	111.3	32.50	0.00		27	34	3.20	2.070	7.62	0.
0.076	0.866	119.6	0.291	159.9	32.50	0.00		17	18	6.50	0.000	6.38	0.
0.082	0.866	110.3	0.291	147.5	32.50	0.00		31	32	5.70	0.000	7.10	0.
0.088	0.866	102.2	0.291	136.7	32.50	0.00		52	53	4.80	0.000	7.73	0.
0.095	0.866	95.1	0.291	127.2	32.50	0.00		36	48	4.10	0.519	7.73	0.
0.102	0.866	88.8	0.291	118.8	32.50	0.00		8	32	4.00	1.845	7.00	0.

RUN NUMBER 336
PREMIXED FLAT FLAME BURNER
STAGED COMBUSTION
METHANE COLD WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STOIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.076	0.866	119.6	0.364	170.0	32.50	0.00		13	14	7.30	0.000	5.87	0.
0.082	0.866	110.3	0.364	156.8	32.50	0.00		28	28	6.40	0.000	6.48	0.
0.088	0.866	102.2	0.364	145.3	32.50	0.00		55	56	5.60	0.000	7.21	0.
0.095	0.866	95.1	0.364	135.2	32.50	0.00		25	42	5.00	0.573	7.21	0.
0.102	0.866	88.8	0.364	126.2	32.50	0.00		7	29	4.80	1.689	6.48	0.
0.076	0.866	119.6	0.438	180.2	32.50	0.00		15	15	7.80	0.000	5.56	0.
0.082	0.866	110.3	0.438	166.2	32.50	0.00		30	30	6.90	0.000	6.28	0.
0.088	0.866	102.2	0.438	154.0	32.50	0.00		53	54	6.10	0.000	6.90	0.
0.095	0.866	95.1	0.438	143.3	32.50	0.00		26	38	5.60	0.546	6.79	0.
0.102	0.866	88.8	0.438	133.8	32.50	0.00		5	25	5.50	1.877	6.07	0.

RUN NUMBER 340
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.018	0.606	345.4	5.95	0.00	1800	3	4	16.00	0.000	3.25	2.
0.023	0.606	269.3	5.95	0.00	1800	4	5	14.80	0.000	3.94	1.
0.028	0.606	219.8	5.95	0.00	1800	6	8	12.90	0.000	4.95	0.
0.034	0.606	184.9	5.95	0.00	1800	13	16	10.90	0.000	5.97	0.
0.040	0.606	159.1	5.95	0.00	1800	27	33	8.90	0.000	6.90	0.
0.045	0.606	139.3	5.95	0.00	1800	56	68	6.60	0.000	7.93	1.
0.051	0.606	123.5	5.95	0.00	1800	97	115	4.70	0.028	8.87	0.
0.057	0.606	110.8	5.95	0.00	1800	150	170	2.60	0.079	9.71	0.
0.063	0.606	100.2	5.95	0.00	1800	160	170	0.90	0.899	10.73	0.
0.051	0.606	123.5	5.95	0.00	1800	140	155	5.10	0.028	8.66	0.

RUN NUMBER 341
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.018	0.606	345.4	1.00	0.00	1540	2	4	14.00	0.028	0.84	3.
0.018	0.606	345.4	1.00	-0.10	1540	1	3	14.00	0.028	0.84	3.
0.018	0.606	345.4	1.00	0.10	1540	1	3	13.50	0.000	0.84	4.
0.016	0.606	345.4	1.00	0.20	1540	1	3	13.00	0.000	0.84	4.
0.018	0.606	345.4	1.00	-0.20	1540	2	3	13.50	0.000	0.84	4.
0.023	0.606	269.3	1.00	-0.20	1540	1	3	13.50	0.079	1.12	5.
0.023	0.606	269.3	1.00	0.00	1540	1	3	13.20	0.104	1.22	5.
0.028	0.606	219.8	1.00	0.00	1540	1	3	12.00	0.232	2.27	5.
0.023	0.606	269.3	1.00	-0.10	1540	1	3	12.40	0.232	1.69	4.
0.023	0.606	269.3	1.00	0.10	1540	1	3	12.00	0.206	1.69	4.
0.023	0.606	269.3	1.00	0.20	1540	1	3	12.60	0.206	1.60	6.
0.023	0.606	269.3	1.00	0.00	1540	1	3	12.90	0.206	1.60	5.
0.023	0.606	269.3	1.00	-0.20	1540	1	3	12.50	0.181	1.50	4.
0.028	0.606	219.8	1.00	-0.10	1540	1	3	11.40	0.258	2.37	4.
0.028	0.606	219.8	1.00	-0.20	1540	1	3	11.10	0.283	2.46	5.
0.028	0.606	219.8	1.00	0.10	1540	1	3	10.80	0.283	2.56	6.
0.028	0.606	219.8	1.00	0.20	1540	1	3	10.90	0.309	2.66	6.
0.028	0.606	219.8	1.00	0.00	1540	1	3	11.40	0.258	2.56	5.
0.034	0.606	184.9	1.00	0.00	1540	1	3	9.60	0.440	3.94	5.
0.034	0.606	184.9	1.00	0.10	1540	1	3	9.10	0.414	4.24	5.
0.034	0.606	184.9	1.00	0.20	1540	1	3	8.80	0.388	4.44	5.
0.034	0.606	184.9	1.00	-0.10	1540	1	4	9.40	0.440	4.04	5.
0.034	0.606	184.9	1.00	-0.20	1540	1	4	9.40	0.440	4.04	5.

RUN NUMBER 341 CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.040	0.606	159.1	1.00	-0.20	1540	2	5	6.80	0.181	5.97	6.
0.040	0.606	159.1	1.00	-0.10	1540	2	5	6.90	0.181	5.97	4.
0.040	0.606	159.1	1.00	0.00	1540	2	5	6.90	0.155	5.97	4.
0.040	0.606	159.1	1.00	0.10	1540	3	5	6.80	0.129	5.97	4.
0.040	0.606	159.1	1.00	0.20	1540	3	5	6.70	0.079	5.87	4.
0.045	0.606	139.3	1.00	0.20	1540	6	8	5.30	0.028	6.90	5.
0.045	0.606	139.3	1.00	0.10	1540	6	8	5.40	0.000	7.00	5.
0.045	0.606	139.3	1.00	0.00	1540	7	9	5.60	0.028	7.00	5.
0.045	0.606	139.3	1.00	-0.10	1540	7	9	5.60	0.028	6.90	4.
0.045	0.606	139.3	1.00	-0.20	1540	7	9	5.50	0.028	6.90	5.
0.051	0.606	123.5	1.00	-0.20	1540	12	15	4.10	0.028	7.73	3.
0.051	0.606	123.5	1.00	-0.10	1540	12	15	4.10	0.053	7.83	4.
0.051	0.606	123.5	1.00	0.00	1540	12	16	4.20	0.053	7.73	4.
0.051	0.606	123.5	1.00	0.10	1540	12	15	4.20	0.028	7.73	5.
0.051	0.606	123.5	1.00	0.20	1540	11	14	4.20	0.028	7.62	5.
0.057	0.606	110.8	1.00	0.20	1540	18	23	2.70	0.079	8.56	5.
0.057	0.606	110.8	1.00	0.10	1540	19	25	2.60	0.079	8.66	5.
0.057	0.606	110.8	1.00	0.00	1540	19	26	2.70	0.129	8.56	6.
0.057	0.606	110.8	1.00	-0.10	1540	19	26	2.60	0.129	8.46	5.
0.057	0.606	110.8	1.00	-0.20	1540	19	27	2.60	0.104	8.56	4.

RUN NUMBER 343
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.063	0.606	100.2	1.00	0.00	1600	27	33	1.50	0.573	9.19	0.
0.063	0.606	100.2	1.00	-0.10	1600	27	33	1.40	0.599	9.19	0.
0.063	0.606	100.2	1.00	0.10	1600	27	34	1.40	0.546	9.19	0.
0.063	0.606	100.2	1.00	0.20	1600	28	35	1.40	0.573	9.08	0.
0.063	0.606	100.2	1.00	-0.20	1600	28	35	1.30	0.653	9.08	0.
0.063	0.606	100.2	0.75	0.00	1600	27	33	1.10	0.816	9.19	0.
0.063	0.606	100.2	0.75	-0.10	1600	27	32	1.10	0.844	9.19	0.
0.063	0.606	100.2	0.75	0.10	1600	28	33	1.10	0.816	9.19	0.
0.063	0.606	100.2	0.75	0.20	1600	28	33	1.10	0.844	9.29	0.
0.063	0.606	100.2	0.75	-0.20	1600	27	32	1.10	0.872	9.08	0.
0.063	0.606	100.2	0.75	0.00	1600	24	29	1.00	0.789	9.29	0.
0.063	0.606	100.2	0.75	-0.10	1600	25	30	1.00	0.816	9.29	0.
0.063	0.606	100.2	0.75	0.10	1600	25	29	0.97	0.872	9.19	0.
0.063	0.606	100.2	0.75	0.20	1600	25	30	0.96	0.872	9.19	0.
0.063	0.606	100.2	0.75	-0.20	1600	25	30	0.97	0.899	9.19	0.
0.063	0.606	100.2	0.25	0.00	1600	22	27	0.97	0.844	9.29	0.
0.063	0.606	100.2	0.25	-0.10	1600	22	27	0.99	0.844	9.29	0.
0.063	0.606	100.2	0.25	0.10	1600	22	26	0.98	0.816	9.29	0.
0.063	0.606	100.2	0.25	0.20	1600	22	27	0.97	0.816	9.08	0.
0.063	0.606	100.2	0.25	-0.20	1600	23	28	0.98	0.816	9.19	0.
0.063	0.606	100.2	0.25	-0.15	1600	23	28	1.10	0.789	9.19	0.
0.063	0.606	100.2	0.25	-0.05	1600	21	26	1.00	0.844	9.19	0.
0.063	0.606	100.2	0.25	0.05	1600	21	26	0.99	0.816	9.29	0.

RUN NUMBER 344
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.123	0.606	51.6	1.00	0.00	1600	1	2	6.00	5.412	2.37	2.
0.123	0.606	51.6	1.00	0.00	1600	1	2	7.40	4.158	1.98	2.
0.123	0.606	51.6	1.00	0.00	1600	0	1	8.50	3.403	1.79	1.
0.109	0.606	58.3	1.00	0.00	1600	1	2	4.20	6.134	3.15	1.
0.109	0.606	58.3	1.00	0.00	1600	1	2	4.50	5.984	3.05	1.
0.116	0.606	54.8	1.00	0.00	1600	1	1	5.40	5.551	2.66	2.
0.116	0.606	54.8	1.00	0.00	1600	1	1	5.90	5.412	2.56	3.
0.123	0.606	51.6	1.00	0.00	1600	1	1	6.60	4.882	2.17	3.
0.123	0.606	51.6	1.00	0.00	1600	1	1	7.40	4.274	1.98	2.
0.109	0.606	58.3	1.00	0.00	1600	1	1	4.60	5.837	2.85	3.
0.109	0.606	58.3	1.00	-0.10	1600	1	1	4.40	5.837	2.85	3.
0.109	0.606	58.3	1.00	0.10	1600	1	1	4.60	5.837	2.85	3.
0.109	0.606	58.3	1.00	0.20	1600	1	1	4.50	5.693	2.85	3.
0.109	0.606	58.3	1.00	-0.20	1600	1	1	4.40	5.984	2.85	4.
0.109	0.606	58.3	1.00	0.00	1600	1	1	5.20	5.412	2.66	4.
0.045	0.606	139.3	1.00	0.00	1600	7	10	5.00	0.079	7.21	5.
0.057	0.606	110.8	1.00	0.00	1600	18	26	2.20	0.206	8.77	6.
0.063	0.606	100.2	1.00	0.00	1600	30	35	1.10	0.816	9.08	6.
0.069	0.606	91.3	1.00	0.00	1600	37		0.82	2.681	8.25	5.
0.076	0.606	83.7	1.00	0.00	1600	34		0.79	4.274	7.10	6.
0.082	0.606	77.2	1.00	0.00	1600	24		0.83	5.693	6.07	6.
0.088	0.606	71.6	1.00	0.00	1600	4		1.30	6.603	5.15	6.
0.095	0.606	66.6	1.00	0.00	1600	1		2.30	6.765	4.14	6.

RUN NUMBER 344 CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.109	0.606	58.3	0.75	-0.10	1600	1	2	5.30	5.551	2.76	9.
0.109	0.606	58.3	0.75	0.10	1600	1	1	5.50	5.412	2.66	9.
0.109	0.606	58.3	0.75	0.20	1600	1	1	5.10	5.551	2.76	9.
0.109	0.606	58.3	0.75	-0.20	1600	1	1	5.60	5.276	2.56	8.
0.109	0.606	58.3	0.50	0.00	1600	1	1	6.30	4.882	2.46	10.
0.109	0.606	58.3	0.50	-0.10	1600	1	2	6.80	4.632	2.27	11.
0.109	0.606	58.3	0.50	0.10	1600	1	2	7.00	4.510	2.37	10.
0.109	0.606	58.3	0.50	0.20	1600	1	2	6.60	4.632	2.37	10.
0.109	0.606	58.3	0.50	-0.20	1600	0	3	7.80	4.158	2.17	11.
0.109	0.606	58.3	0.25	0.00	1600	0	3	7.90	4.882	2.85	0.
0.109	0.606	58.3	0.25	0.00	1600	0	1	10.70	2.817	2.27	0.

RUN NUMBER 347
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.063	0.606	100.2	1.00	0.00	1450	24	30	1.20	0.335	9.19	0.
0.067	0.606	94.7	1.00	0.00	1450	34		0.82	1.269	8.87	0.
0.069	0.606	91.3	1.00	0.00	1450	37		0.79	2.135	8.46	0.
0.073	0.606	86.6	1.00	0.00	1450	38		0.81	2.824	8.04	0.
0.076	0.606	83.7	1.00	0.00	1450	38		0.84	3.716	7.42	0.
0.082	0.606	77.2	1.00	0.00	1450	27		0.88	5.276	6.38	0.
0.088	0.606	71.6	1.00	0.00	1450	13		1.20	6.444	5.25	0.
0.095	0.606	66.6	1.00	0.00	1450	1	5	2.50	6.765	4.34	0.
0.102	0.606	62.2	1.00	0.00	1450	0	3	6.60	5.142	3.05	0.

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                                  RUN NUMBER  349
                            ADIABATIC STIRRED COMBUSTOR
                                NORMAL COMBUSTION
                              PROPANE      HOT  WALL

FUEL     AIR      PCT      AXIAL   RADIAL   WALL     NO       NOX      O2      CO       CO2      HC
FLOW     FLOW     STOIC    DIST    DIST     TEMP
(CFM)    (CFM)    AIR      (IN)    (IN)     (C)      (PPM)    (PPM)    (PCT)   (PCT)    (PCT)    (PPM)


0.017    0.594    141.9    0.15     0.00    1600       8       11      8.30    0.000    7.10       5.
0.017    0.594    141.9    0.15    -0.08    1600       8       11      8.40    0.000    7.00       0.
0.017    0.594    141.9    0.15    -0.15    1600       7       11      8.50    0.000    6.90       0.
0.017    0.594    141.9    0.15    -0.23    1600       7       10      8.40    0.000    6.79       0.
0.017    0.594    141.9    0.15    -0.30    1600       8       11      8.20    0.000    7.00       0.
0.017    0.594    141.9    0.15     0.08    1600       9       12      8.20    0.000    7.00       0.
0.017    0.594    141.9    0.15     0.15    1600       9       12      8.40    0.000    6.90       0.
0.017    0.594    141.9    0.15     0.23    1600       8       11      8.30    0.000    6.90       0.
0.017    0.594    141.9    0.15     0.30    1600       8       11      8.30    0.000    6.90       0.
0.017    0.594    141.9    0.05     0.00    1600       9       12      8.20    0.000    6.79       0.
0.017    0.594    141.9    0.05    -0.08    1600       9       12      7.90    0.000    6.79       0.
0.017    0.594    141.9    0.05    -0.15    1600       8       11      8.10    0.000    6.69       0.
0.017    0.594    141.9    0.05    -0.23    1600       8       11      8.00    0.000    6.59       0.
0.017    0.594    141.9    0.05    -0.30    1600       7       10      8.20    0.000    6.48       0.
0.017    0.594    141.9    0.05     0.08    1600       8       10      8.20    0.000    6.48       0.
0.017    0.594    141.9    0.05     0.15    1600       7       10      8.10    0.000    6.59       0.
0.017    0.594    141.9    0.05     0.23    1600       8       10      8.10    0.000    6.59       0.
0.017    0.594    141.9    0.05     0.30    1600       7       10      8.00    0.000    6.59       0.
0.017    0.594    141.9    0.25     0.00    1600       7        9      8.10    0.000    6.59       0.
0.017    0.594    141.9    0.25    -0.15    1600       7        9      8.00    0.000    6.59       0.
0.017    0.594    141.9    0.25    -0.30    1600       6        8      8.00    0.000    6.69       0.
0.017    0.594    141.9    0.25     0.15    1600       7        9      8.10    0.000    6.59       0.
0.017    0.594    141.9    0.25     0.30    1600       6        8      8.00    0.000    6.59       0.
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RUN NUMBER 350
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.017	0.594	141.9	0.50	0.00	1600	4	6	9.60	0.000	6.59	0.
0.017	0.594	141.9	0.50	-0.15	1600	4	6	9.60	0.000	6.69	0.
0.017	0.594	141.9	0.50	-0.30	1600	4	6	9.60	0.000	6.59	0.
0.017	0.594	141.9	0.50	0.15	1600	5	7	9.90	0.000	6.48	0.
0.017	0.594	141.9	0.50	0.30	1600	4	6	9.70	0.000	6.48	0.
0.017	0.594	141.9	0.75	0.00	1600	4	6	9.60	0.000	6.59	0.
0.017	0.594	141.9	0.75	-0.15	1600	4	6	9.60	0.000	6.48	0.
0.017	0.594	141.9	0.75	-0.30	1600	4	6	9.40	0.000	6.69	0.
0.017	0.594	141.9	0.75	0.15	1600	5	7	9.40	0.000	6.69	0.
0.017	0.594	141.9	0.75	0.30	1600	4	6	9.20	0.000	6.69	0.
0.017	0.594	141.9	1.00	0.00	1600	4	6	9.40	0.000	6.69	0.
0.017	0.594	141.9	1.00	-0.15	1600	4	6	9.20	0.000	6.59	0.
0.017	0.594	141.9	1.00	-0.30	1600	5	7	9.40	0.000	6.59	0.
0.017	0.594	141.9	1.00	0.15	1600	5	7	9.60	0.000	6.48	0.
0.017	0.594	141.9	1.00	0.30	1600	4	6	9.50	0.000	6.38	0.
0.017	0.594	141.9	2.00	0.00	1600	7	9	8.10	0.000	7.31	0.
0.017	0.594	141.9	3.00	0.00	1600	9	11	8.10	0.000	7.31	0.
0.017	0.594	141.9	4.00	0.00	1600	10	12	8.00	0.000	7.21	0.
0.017	0.594	141.9	5.00	0.00	1600	11	13	8.10	0.000	7.00	0.
0.017	0.594	141.9	6.00	0.00	1600	12	14	8.10	0.000	7.10	0.
0.017	0.594	141.9	0.05	0.00	1600	5	7	7.90	0.000	7.31	0.
0.017	0.594	141.9	-0.05	-0.15	1600	4	6	8.00	0.000	7.31	0.
0.017	0.594	141.9	0.05	-0.30	1600	4	6	7.90	0.000	7.21	0.

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                                   RUN NUMBER  350 CONT
                              ADIABATIC STIRRED COMBUSTOR
                                  NORMAL COMBUSTION
                                 PROPANE      HOT  WALL

FUEL     AIR      PCT     AXIAL   RADIAL    WALL     NO       NOX       O2       CO       CO2      HC
FLOW     FLOW     STOIC   DIST    DIST      TEMP
(CFM)    (CFM)    AIR     (IN)    (IN)      (C)     (PPM)    (PPM)    (PCT)    (PCT)    (PCT)    (PPM)


0.017    0.594    141.9   0.05     0.15     1600        4        6     8.00     0.000    7.31        0.
0.017    0.594    141.9   0.05     0.30     1600        4        5     7.80     0.000    7.21        0.
0.022    0.594    112.4   0.05     0.00     1600        6        8     4.00     0.000    9.60        0.
0.022    0.594    112.4   0.05    -0.15     1600        6        9     4.20     0.000    9.50        0.
0.022    0.594    112.4   0.05    -0.30     1600        7        9     4.10     0.000    9.50        0.
0.022    0.594    112.4   0.05     0.15     1600        7        9     4.20     0.000    9.39        0.
0.022    0.594    112.4   0.05     0.30     1600        6        9     4.50     0.028    9.29        0.
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                          RUN NUMBER  351
                     ADIABATIC STIRRED COMBUSTOR
                         NORMAL COMBUSTION
                        PROPANE     HOT  WALL

FUEL     AIR      PCT      AXIAL   RADIAL    WALL     NO       NOX      O2       CO       CO2      HC
FLOW     FLOW     STOIC    DIST    DIST      TEMP
(CFM)    (CFM)    AIR      (IN)    (IN)      (C)      (PPM)    (PPM)    (PCT)    (PCT)    (PCT)    (PPM)


0.011    0.594    219.1     3.20     0.00    1600        2        4    14.00    0.000     4.55       0.
0.011    0.438    161.7     3.20     0.00    1600        6        9    10.50    0.000     6.28       0.
0.031    0.678     90.8     3.20     0.00    1600       41       42     1.45    2.201     9.50       0.
0.024    0.678    117.3     3.20     0.00    1600       17       23     4.80    0.000     9.39       0.
0.017    0.678    161.8     3.20     0.00    1600        5        8     9.70    0.000     6.90       0.
0.011    0.678    249.9     3.20     0.00    1600        3        5    14.40    0.000     4.34       0.
0.005    0.678    498.7     3.20     0.00    1600        1        3    20.00    0.206     1.31    1600.
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RUN NUMBER 352*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.012	0.678	226.1	3.20	0.00	1600	3	4	13.90	0.000	4.55	0.
0.015	0.678	189.1	3.20	0.00	1600	3	5	12.30	0.000	5.25	0.
0.017	0.678	161.8	3.20	0.00	1600	5	7	10.70	0.000	6.07	0.
0.020	0.678	140.9	3.20	0.00	1600	9	11	8.60	0.000	7.10	0.
0.022	0.678	124.3	3.20	0.00	1600	24	30	6.20	0.000	8.35	0.
0.024	0.678	114.1	3.20	0.00	1600	43	53	5.00	0.000	8.87	0.
0.027	0.678	105.2	3.20	0.00	1600	19	26	3.40	0.053	9.60	0.
0.029	0.678	97.5	3.20	0.00	1600	38	42	1.80	0.872	10.49	0.
0.031	0.678	90.8	3.20	0.00	1600	44	45	1.70	3.104	9.02	0.
0.035	0.678	79.5	3.20	0.00	1600	46	46	1.60	5.837	7.13	0.
0.038	0.678	73.3	3.20	0.00	1600	46		1.60	7.810	6.21	0.
0.035	0.678	79.5	3.20	-0.15	1600	44	44	1.60	5.984	7.36	0.
0.035	0.678	79.5	3.20	-0.30	1600	45	45	1.55	5.837	7.13	0.
0.035	0.678	79.5	3.20	0.15	1600	44	44	1.50	5.984	7.36	0.
0.035	0.678	79.5	3.20	0.30	1600	43	43	1.50	5.984	7.36	0.
0.044	0.678	64.3	3.20	0.00	1600	18		1.45	7.448	5.53	400.
0.046	0.678	61.1	3.20	0.00	1600	2		1.40	9.626	5.08	7500.
0.049	0.678	58.1	3.20	0.00	1600	1		1.40	11.023	4.20	10000.
0.050	0.678	56.3	3.20	0.00	1600	1		1.40	11.023	4.20	18000.
0.017	0.678	161.8	3.20	-0.15	1600	6	10	9.90	0.000	6.90	0.
0.017	0.678	161.8	3.20	-0.30	1600	4	7	9.80	0.000	6.69	0.
0.017	0.678	161.8	3.20	0.15	1600	5	7	9.90	0.000	6.79	0.
0.017	0.678	161.8	3.20	0.30	1600	4	6	9.80	0.000	6.69	0.

* Air leak in sampling system amounting to 8% of total sampled volume.

RUN NUMBER 352* CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.017	0.678	161.8	2.20	0.00	1600	3	6	9.90	0.000	6.69	0.
0.035	0.678	79.5	2.20	0.00	1600	43	43	1.50	5.693	7.93	0.
0.035	0.678	79.5	1.20	0.00	1600	40		1.40	5.551	8.14	0.

* Air leak in sampling system amounting to 8% of total sampled volume.

RUN NUMBER 353*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.017	0.678	161.8	1.20	0.00	1600	4	6	10.70	0.028	6.59	0.
0.017	0.678	161.8	1.00	0.00	1600	4	6	10.80	0.000	6.48	0.
0.017	0.678	161.8	1.00	-0.15	1600	4	6	10.80	0.028	6.48	0.
0.017	0.678	161.8	1.00	-0.30	1600	4	5	10.70	0.028	6.38	0.
0.017	0.678	161.8	1.00	0.15	1600	4	6	10.70	0.000	6.48	0.
0.017	0.678	161.8	1.00	0.30	1600	4	6	10.60	0.028	6.38	0.
0.035	0.678	79.5	1.00	0.00	1600	38	39	1.60	4.274	8.46	0.
0.035	0.678	79.5	1.00	-0.15	1600	37	38	1.60	4.632	8.25	0.
0.035	0.678	79.5	1.00	-0.30	1600	38	39	1.70	4.756	8.14	0.
0.035	0.678	79.5	1.00	0.15	1600	36	37	1.60	4.632	8.14	0.
0.035	0.678	79.5	1.00	0.30	1600	39	40	1.70	4.882	7.83	0.
0.035	0.678	79.5	0.75	0.00	1600	40	-	1.50	5.984	7.42	0.
0.035	0.678	79.5	0.75	-0.15	1600	41	-	1.60	5.984	7.42	0.
0.035	0.678	79.5	0.75	-0.30	1600	41	-	1.60	5.984	7.31	0.
0.035	0.678	79.5	0.75	0.15	1600	39	-	1.50	5.837	7.52	0.
0.035	0.678	79.5	0.75	0.30	1600	40	-	1.60	5.837	7.31	0.
0.017	0.678	161.8	0.75	0.00	1600	5	7	10.40	0.028	6.59	0.
0.017	0.678	161.8	0.75	-0.15	1600	4	7	10.30	0.000	6.69	0.
0.017	0.678	161.8	0.75	-0.30	1600	4	6	10.20	0.000	6.59	0.
0.017	0.678	161.8	0.75	0.15	1600	4	6	10.20	0.000	6.48	0.
0.017	0.675	161.8	0.75	0.30	1600	3	6	10.00	0.000	6.38	0.
0.017	0.678	161.8	0.50	0.00	1600	3	6	10.10	0.000	6.48	0.
0.017	0.678	161.8	0.50	-0.15	1600	3	5	10.20	0.000	6.48	0.

* Air leak in sampling system amounting to 8% of sampled volume.

RUN NUMBER 353* CONT
ADIABATIC STIRRED CCMBUSTCR
NORMAL CCMBUSTICN
PRCPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RACIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	C2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.017	0.678	161.8	0.50	-0.30	1600	3	5	10.00	0.00C	6.38	0.
0.017	0.678	161.8	0.50	0.15	1600	4	6	9.90	0.00C	6.48	0.
0.017	0.678	161.8	0.50	0.3C	1600	3	6	9.80	0.00C	6.38	0.
0.035	0.678	79.5	0.50	C.CC	1600	34	-	1.40	4.51C	8.14	C.
0.035	0.678	79.5	0.50	-C.15	1600	35	-	1.30	4.756	8.04	0.
0.035	C.678	79.5	0.50	-C.3C	1600	33	-	1.40	4.632	8.C4	C.
0.035	0.678	79.5	0.50	0.15	16C0	33	-	1.40	5.142	7.83	C.
0.035	0.678	79.5	0.50	0.30	1600	33	-	1.40	5.412	7.52	C.
0.035	0.678	79.5	0.25	C.0C	16C0	29	-	1.30	5.142	7.93	0.
0.035	0.678	79.5	0.25	-0.15	1600	30	-	1.30	5.276	7.83	0.
0.035	0.678	79.5	0.25	-0.30	1600	29	-	1.40	5.551	7.62	0.
0.035	0.678	79.5	0.25	0.15	1600	29	-	1.30	5.693	7.62	0.
0.035	0.678	79.5	0.25	0.30	1600	28	-	1.30	5.693	7.52	0.
0.017	0.678	161.8	C.25	0.0C	16C0	5	7	1C.00	C.028	6.69	0.
0.017	0.678	161.8	0.25	-C.15	16C0	4	7	9.70	0.0CC	6.79	0.
0.017	0.678	161.8	0.25	-C.3C	16C0	5	7	9.50	0.028	6.79	0.
0.017	C.678	161.8	0.25	C.15	16C0	5	7	9.50	0.00C	6.90	0.
0.017	0.678	161.8	0.25	0.30	1600	5	7	9.40	0.00C	6.69	0.

* Air leak in sampling system amounting to 8% of sampled volume.

RUN NUMBER 354*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.017	0.678	161.8	0.05	0.00	1600	4	6	9.60	0.028	6.69	5.
0.017	0.678	161.8	0.05	-0.15	1600	3	4	9.50	0.053	6.79	30.
0.017	0.678	161.8	0.05	-0.30	1600	3	5	9.40	0.053	6.69	10.
0.017	0.678	161.8	0.05	0.15	1600	4	6	9.40	0.028	6.79	0.
0.017	0.678	161.8	0.05	0.30	1600	4	5	9.30	0.028	6.59	0.
0.035	0.678	79.5	0.05	0.00	1600	36	-	1.10	5.011	8.46	0.
0.035	0.678	79.5	0.05	-0.15	1600	37	-	1.20	5.412	8.14	0.
0.035	0.678	79.5	0.05	-0.30	1600	38	-	1.20	5.276	8.04	0.
0.035	0.678	79.5	0.05	0.15	1600	36	-	1.10	5.142	8.25	0.
0.035	0.678	79.5	0.05	0.30	1600	37	-	1.20	4.756	8.25	0.
0.012	0.678	226.1	0.05	0.00	1600	0	2	14.60	0.440	3.94	6800.
0.015	0.678	189.1	0.05	0.00	1600	0	3	11.80	0.155	5.46	1000.
0.017	0.678	161.8	0.05	0.00	1600	4	7	9.30	0.028	6.90	10.
0.020	0.678	140.9	0.05	0.00	1600	8	11	7.80	0.053	7.52	0.
0.022	0.678	124.3	0.05	0.00	1600	26	36	5.40	0.129	8.66	0.
0.024	0.678	114.1	0.05	0.00	1600	9	14	4.50	0.104	9.29	0.
0.027	0.678	105.2	0.05	0.00	1600	16	22	2.50	0.129	10.49	0.
0.029	0.678	97.5	0.05	0.00	1600	29	32	1.20	1.240	10.73	0.
0.031	0.678	90.8	0.05	0.00	1600	34	35	1.10	3.506	9.19	0.
0.035	0.678	79.5	0.05	0.00	1600	37	-	1.10	4.882	8.25	0.
0.038	0.678	73.3	0.05	0.00	1600	35	-	1.10	6.765	7.21	10.
0.041	0.678	67.9	0.05	0.00	1600	26	-	1.10	9.408	5.46	3500.

* Air leak in sampling system amounting to 5% of sampled volume.

RUN NUMBER 359*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.020	0.678	140.9	0.25	-0.30	1600	7	9	8.10	0.028	7.31	0.
0.020	0.678	140.9	0.25	-0.15	1600	8	11	8.10	0.028	7.42	0.
0.020	0.678	140.9	0.50	-0.15	1600	9	12	7.90	0.000	7.52	0.
0.020	0.678	140.9	0.50	-0.30	1600	8	12	7.80	0.028	7.42	0.
0.020	0.678	140.9	0.75	-0.30	1600	8	12	7.80	0.028	7.42	0.
0.020	0.678	140.9	0.75	-0.15	1600	10	13	7.90	0.000	7.52	0.
0.020	0.678	140.9	1.00	-0.15	1600	10	13	7.80	0.000	7.52	0.
0.020	0.678	140.9	1.00	-0.30	1600	9	13	7.80	0.000	7.42	0.
0.024	0.678	114.1	0.25	-0.30	1600	10	15	4.30	0.181	9.29	0.
0.024	0.678	114.1	0.25	-0.15	1600	10	15	4.40	0.155	9.29	0.
0.024	0.678	114.1	0.50	-0.15	1600	11	16	4.30	0.125	9.39	0.
0.024	0.678	114.1	0.50	-0.30	1600	12	16	4.20	0.155	9.29	0.
0.024	0.678	114.1	0.75	-0.30	1600	11	15	4.20	0.155	9.19	0.
0.024	0.678	114.1	0.75	-0.15	1600	12	17	4.10	0.104	9.39	0.
0.024	0.678	114.1	1.00	-0.15	1600	12	16	4.20	0.079	9.39	0.

* Air leak in sampling system amounting to 5% of sampled volume.

RUN NUMBER 355*CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.024	0.678	114.1	1.00	-0.30	1600	11	16	4.30	0.104	9.19	0.
0.027	0.678	105.2	0.25	-0.30	1600	15	25	2.10	0.309	9.71	0.
0.027	0.678	105.2	0.25	-0.15	1600	14	24	2.10	0.361	10.49	0.
0.027	0.678	105.2	0.50	-0.15	1600	16	26	2.10	0.361	10.73	0.
0.027	0.678	105.2	0.50	-0.30	1600	14	25	2.40	0.309	9.92	0.
0.027	0.678	105.2	0.75	-0.30	1600	16	26	2.50	0.283	9.92	0.
0.027	0.678	105.2	0.75	-0.15	1600	17	26	2.20	0.206	10.73	0.
0.027	0.678	105.2	1.00	-0.15	1600	19	28	2.20	0.283	10.49	0.
0.027	0.678	105.2	1.00	-0.30	1600	19	28	2.10	0.335	10.49	0.
0.029	0.678	97.5	0.25	-0.30	1600	29	34	1.00	1.096	10.49	0.
0.029	0.678	97.5	0.25	-0.15	1600	25	31	1.10	0.734	11.23	0.
0.029	0.678	97.5	0.50	-0.15	1600	26	32	1.00	0.707	10.98	0.
0.029	0.678	97.5	0.50	-0.30	1600	26	32	1.00	1.068	10.73	0.
0.029	0.678	97.5	0.75	-0.30	1600	30	34	1.10	1.476	10.49	0.
0.029	0.678	97.5	0.75	-0.15	1600	32	35	0.90	1.506	10.49	0.
0.029	0.678	97.5	1.00	-0.15	1600	32	34	0.90	1.567	10.49	0.
0.029	0.678	97.5	1.00	-0.30	1600	32	35	1.00	1.659	10.49	0.
0.031	0.678	90.8	0.25	-0.30	1600	32	33	0.82	2.681	9.60	0.
0.031	0.678	90.8	0.25	-0.15	1600	29	30	0.79	2.681	9.71	0.
0.031	0.678	90.8	0.50	-0.15	1600	31	32	0.81	2.788	9.60	0.
0.031	0.678	90.8	0.50	-0.30	1600	32	33	0.83	2.752	9.39	0.
0.031	0.678	90.8	0.75	-0.30	1600	33	34	0.90	2.933	9.39	0.
0.031	0.678	90.8	0.75	-0.15	1600	34	36	0.90	2.912	9.50	0.

* Air leak in sampling system amounting to 5% of sampled volume.

RUN NUMBER 355*CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.031	0.678	90.8	1.00	-0.15	1600	36	-	0.92	3.007	9.39	0.
0.031	0.678	90.8	1.00	-0.30	1600	36	-	0.92	3.007	9.19	0.
0.035	0.678	79.5	0.25	-0.30	1600	34	-	0.84	5.693	7.62	0.
0.035	0.678	79.5	0.25	-0.15	1600	32	-	0.80	5.693	7.83	0.
0.035	0.678	79.5	0.50	-0.15	1600	34	-	0.82	5.837	7.42	0.
0.035	0.678	79.5	0.50	-0.30	1600	36	-	0.84	5.837	7.62	0.
0.035	0.678	79.5	0.75	-0.30	1600	36	-	0.87	5.837	7.52	0.
0.035	0.678	79.5	0.75	-0.15	1600	36	-	0.84	5.837	7.62	0.
0.035	0.678	79.5	1.00	-0.15	1600	37	-	0.83	5.984	7.52	0.
0.035	0.678	79.5	1.00	-0.30	1600	38	-	0.86	5.984	7.52	0.
0.038	0.678	73.3	0.25	-0.30	1600	22	-	0.81	7.627	6.59	920.
0.038	0.678	73.3	0.25	-0.15	1600	18	-	0.82	7.810	6.69	1600.
0.038	0.678	73.3	0.50	-0.15	1600	21	-	0.79	7.627	6.69	600.
0.038	0.678	73.3	0.50	-0.30	1600	26	-	0.82	7.627	6.59	270.
0.038	0.678	73.3	0.75	-0.30	1600	32	-	0.83	7.996	6.48	20.
0.038	0.678	73.3	0.75	-0.15	1600	28	-	0.80	7.810	6.69	240.
0.038	0.678	73.3	1.00	-0.15	1600	32	-	0.80	7.996	6.69	5.
0.038	0.678	73.3	1.00	-0.30	1600	35	-	0.80	7.996	6.38	0.

* Air leak in sampling system amounting to 5% of sampled volume.

RUN NUMBER 356*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.020	0.678	140.9	0.25	0.30	1600	2	5	7.50	0.000	7.62	15.
0.024	0.678	114.1	0.25	0.30	1600	11	16	3.70	0.000	9.39	0.
0.027	0.678	105.2	0.25	0.30	1600	17	23	2.20	0.028	10.49	0.
0.029	0.678	97.5	0.25	0.30	1600	25	29	1.00	0.546	10.73	0.
0.031	0.678	90.8	0.25	0.30	1600	29	31	0.86	3.007	9.29	0.
0.035	0.678	79.5	0.25	0.30	1600	34	-	0.84	5.837	7.62	0.
0.038	0.678	73.3	0.25	0.30	1600	29	-	0.82	7.627	6.59	220.
0.020	0.678	140.9	0.25	0.00	1600	1	5	8.30	0.155	7.00	650.
0.020	0.678	140.9	0.50	0.00	1600	3	6	8.20	0.028	7.21	50.
0.020	0.678	140.9	0.75	0.00	1600	4	7	8.10	0.000	7.31	5.
0.020	0.678	140.9	1.00	0.00	1600	5	8	8.10	0.000	7.31	5.
0.022	0.678	124.3	0.25	0.00	1600	6	11	5.50	0.053	8.66	30.
0.022	0.678	124.3	0.50	0.00	1600	8	13	5.60	0.028	8.77	5.
0.022	0.678	124.3	0.75	0.00	1600	10	17	5.60	0.028	8.66	0.
0.022	0.678	124.3	1.00	0.00	1600	13	19	5.70	0.028	8.56	0.
0.024	0.678	114.1	0.25	0.00	1600	9	13	3.90	0.000	9.50	0.
0.024	0.678	114.1	0.50	0.00	1600	9	13	4.10	0.000	9.39	0.
0.024	0.678	114.1	0.75	0.00	1600	10	14	4.10	0.000	9.39	0.
0.024	0.678	114.1	1.00	0.00	1600	11	15	3.90	0.000	9.50	0.
0.027	0.678	105.2	0.25	0.00	1600	15	21	2.60	0.053	10.49	0.
0.027	0.678	105.2	0.50	0.00	1600	14	21	2.70	0.079	4.55	0.
0.027	0.678	105.2	0.75	0.00	1600	15	22	2.60	0.104	4.55	0.

* Air leak in sampling system amounting to 4% of sampled volume.

RUN NUMBER 356*CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.027	0.678	105.2	1.00	0.00	1600	15	22	2.50	0.129	10.49	0.
0.029	0.678	97.5	0.25	0.00	1600	28	31	0.89	0.927	10.98	0.
0.029	0.678	97.5	0.50	0.00	1600	28	30	0.86	0.844	11.23	0.
0.029	0.678	97.5	0.75	0.00	1600	28	30	0.90	0.899	11.23	0.
0.029	0.678	97.5	1.00	0.00	1600	29	31	0.93	0.983	10.98	0.
0.031	0.678	90.8	0.25	0.00	1600	28	-	0.75	3.104	9.50	0.
0.031	0.678	90.8	0.50	0.00	1600	29	-	0.76	3.104	9.50	0.
0.031	0.678	90.8	0.75	0.00	1600	31	-	0.78	3.203	9.39	0.
0.031	0.678	90.8	1.00	0.00	1600	32	-	0.80	3.302	9.29	0.
0.035	0.678	79.5	0.25	0.00	1600	31	-	0.72	5.837	7.93	0.
0.035	0.678	79.5	0.50	0.00	1600	33	-	0.74	5.693	7.93	0.
0.035	0.678	79.5	0.75	0.00	1600	34	-	0.76	5.837	7.83	0.
0.035	0.678	79.5	1.00	0.00	1600	35	-	0.79	5.984	7.73	0.
0.038	0.678	73.3	0.25	0.00	1600	28	-	0.72	7.996	6.69	140.
0.038	0.678	73.3	0.50	0.00	1600	29	-	0.71	7.996	6.69	100.
0.038	0.678	73.3	0.75	0.00	1600	31	-	0.75	7.996	6.59	70.
0.038	0.678	73.3	1.00	0.00	1600	33	-	0.77	7.996	6.59	25.
0.020	0.678	140.9	0.05	0.30	1600	3	6	7.60	0.000	7.52	15.
0.020	0.678	140.9	0.05	0.15	1600	4	7	7.80	0.000	7.62	10.
0.020	0.678	140.9	0.25	0.15	1600	4	7	7.70	0.000	7.73	5.
0.020	0.678	140.9	0.50	0.30	1600	5	7	7.60	0.000	7.52	0.
0.020	0.678	140.9	0.50	0.15	1600	4	7	7.80	0.000	7.73	0.
0.020	0.678	140.9	0.75	0.15	1600	4	7	7.80	0.000	7.62	0.

* Air leak in sampling system amounting to 4% of sampled volume.

RUN NUMBER 356*CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.020	0.678	140.9	0.75	0.30	1600	4	7	7.70	0.000	7.42	0.
0.020	0.678	140.9	1.00	0.30	1600	5	7	7.80	0.000	7.42	0.
0.020	0.678	140.9	1.00	0.15	1600	5	8	7.80	0.000	7.52	0.
0.024	0.678	114.1	0.05	0.30	1600	9	13	3.90	0.000	9.29	0.
0.024	0.678	114.1	0.05	0.15	1600	9	13	4.00	0.000	9.39	0.
0.024	0.678	114.1	0.25	0.15	1600	10	14	4.00	0.000	9.60	0.
0.024	0.678	114.1	0.50	0.30	1600	11	14	4.10	0.000	9.29	0.
0.024	0.678	114.1	0.50	0.15	1600	10	14	4.20	0.000	9.50	0.
0.024	0.678	114.1	0.75	0.15	1600	10	14	4.20	0.000	9.50	0.
0.024	0.678	114.1	0.75	0.30	1600	11	14	3.90	0.000	9.50	0.
0.024	0.678	114.1	1.00	0.30	1600	11	15	3.90	0.000	9.50	0.
0.024	0.678	114.1	1.00	0.15	1600	12	16	4.00	0.000	9.60	0.

* Air leak in sampling system amounting to 4% of sampled volume.

RUN NUMBER 357
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.027	0.678	105.2	0.05	0.30	1600	16	22	2.40	0.079	10.24	0.
0.027	0.678	105.2	0.05	0.15	1600	16	23	2.30	0.053	10.49	0.
0.027	0.678	105.2	0.25	0.15	1600	17	23	2.20	0.028	10.73	0.
0.027	0.678	105.2	0.50	0.30	1600	18	24	2.30	0.000	10.49	0.
0.027	0.678	105.2	0.50	0.15	1600	17	23	2.40	0.028	10.73	0.
0.027	0.678	105.2	0.75	0.15	1600	16	22	2.40	0.000	10.73	0.
0.027	0.678	105.2	0.75	0.30	1600	17	23	2.30	0.028	10.49	0.
0.027	0.678	105.2	1.00	0.30	1600	17	23	2.50	0.053	10.49	0.
0.027	0.678	105.2	1.00	0.15	1600	16	23	2.50	0.053	10.73	0.
0.029	0.678	97.5	0.05	0.30	1600	26	29	0.78	0.872	10.73	0.
0.029	0.678	97.5	0.05	0.15	1600	25	28	0.80	0.816	10.98	0.
0.029	0.678	97.5	0.25	0.15	1600	26	28	0.76	0.789	11.23	0.
0.029	0.678	97.5	0.50	0.30	1600	26	27	0.78	0.844	10.98	0.
0.029	0.678	97.5	0.50	0.15	1600	27	28	0.74	0.816	10.98	0.
0.029	0.678	97.5	0.75	0.15	1600	27	29	0.80	0.844	11.23	0.
0.029	0.678	97.5	0.75	0.30	1600	26	28	0.82	0.872	10.98	0.
0.029	0.678	97.5	1.00	0.30	1600	27	29	0.83	0.899	10.98	0.
0.029	0.678	97.5	1.00	0.15	1600	27	29	0.80	0.899	11.23	0.
0.031	0.678	90.8	0.05	0.30	1600	29	30	0.73	3.007	9.39	0.
0.031	0.678	90.8	0.05	0.15	1600	28	29	0.71	3.104	9.50	0.
0.031	0.678	90.8	0.25	0.15	1600	27	28	0.70	3.104	9.60	0.
0.031	0.678	90.8	0.50	0.30	1600	28	28	0.73	3.104	9.39	0.

RUN NUMBER 358
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.031	0.678	90.8	0.50	0.15	1600	29	-	0.69	3.203	9.39	0.
0.031	0.678	90.8	0.75	0.15	1600	29	-	0.74	3.302	9.29	0.
0.031	0.678	90.8	0.75	0.30	1600	30	-	0.76	3.302	9.08	0.
0.031	0.678	90.8	1.00	0.30	1600	29	-	0.77	3.403	8.98	0.
0.031	0.678	90.8	1.00	0.15	1600	31	-	0.76	3.403	9.08	0.
0.035	0.678	79.5	0.05	0.30	1600	37	-	0.74	5.837	7.42	0.
0.035	0.678	79.5	0.05	0.15	1600	36	-	0.72	5.984	7.52	0.
0.035	0.678	79.5	0.25	0.15	1600	36	-	0.68	6.134	7.52	0.
0.035	0.678	79.5	0.50	0.30	1600	35	-	0.72	5.984	7.42	0.
0.035	0.678	79.5	0.50	0.15	1600	35	-	0.67	6.134	7.62	0.
0.035	0.678	79.5	0.75	0.15	1600	36	-	0.70	6.134	7.62	0.
0.035	0.678	79.5	0.75	0.30	1600	34	-	0.67	5.984	7.31	0.
0.035	0.678	79.5	1.00	0.30	1600	35	-	0.68	6.134	7.31	0.
0.035	0.678	79.5	1.00	0.15	1600	36	-	0.66	6.134	7.52	0.
0.038	0.678	73.3	0.05	0.30	1600	33	-	0.66	7.448	6.48	160.
0.038	0.678	73.3	0.05	0.15	1600	31	-	0.67	7.448	6.59	250.
0.038	0.678	73.3	0.25	0.15	1600	31	-	0.65	7.627	6.69	130.
0.038	0.678	73.3	0.50	0.30	1600	32	-	0.66	7.448	6.48	40.
0.038	0.678	73.3	0.50	0.15	1600	32	-	0.67	7.627	6.69	45.
0.038	0.678	73.3	0.75	0.15	1600	32	-	0.69	7.627	6.69	25.
0.038	0.678	73.3	0.75	0.30	1600	31	-	0.66	7.627	6.59	30.
0.038	0.678	73.3	1.00	0.30	1600	33	-	0.70	7.810	6.38	5.
0.038	0.678	73.3	1.00	0.15	1600	32	-	0.67	7.810	6.59	25.

RUN NUMBER 358 CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.020	0.678	140.9	0.05	-0.15	1600	5	7	7.50	0.000	7.62	0.
0.020	0.678	140.9	0.05	-0.30	1600	4	7	7.40	0.000	7.62	0.
0.024	0.678	114.1	0.05	-0.15	1600	10	13	4.30	0.000	9.19	0.
0.024	0.678	114.1	0.05	-0.30	1600	9	13	4.30	0.000	9.08	0.
0.027	0.678	105.2	0.05	-0.30	1600	14	20	2.30	0.104	10.24	0.
0.027	0.678	105.2	0.05	-0.15	1600	15	22	2.30	0.079	10.49	0.
0.029	0.678	97.5	0.05	-0.15	1600	25	31	1.00	0.414	10.98	0.
0.029	0.678	97.5	0.05	-0.30	1600	24	29	1.10	0.414	10.73	0.
0.031	0.678	90.8	0.05	-0.30	1600	31	34	0.70	2.541	9.39	0.
0.031	0.678	90.8	0.05	-0.15	1600	30	32	0.69	2.817	9.50	0.
0.035	0.678	79.5	0.05	-0.15	1600	35	-	0.66	5.551	7.73	0.
0.035	0.678	79.5	0.05	-0.30	1600	34	-	0.66	5.412	7.73	0.
0.038	0.678	73.3	0.05	-0.30	1600	31	-	0.65	7.272	6.79	90.
0.038	0.678	73.3	0.05	-0.15	1600	30	-	0.64	7.272	6.79	45.

RUN NUMBER 359
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.000	0.678	*****	1.00	0.00	1800	120	-	20.80	0.000	0.00	0.
0.029	0.678	97.5	1.00	0.00	1800	36	37	0.75	1.269	10.49	0.
0.031	0.678	90.8	1.00	0.00	1800	38	-	0.69	3.007	9.19	0.
0.035	0.678	79.5	1.00	0.00	1800	41	-	0.66	6.134	7.42	0.
0.038	0.678	73.3	1.00	0.00	1800	40	-	0.65	7.627	6.59	0.
0.041	0.678	67.9	1.00	0.00	1800	16	-	0.66	9.194	5.56	1600.
0.000	0.678	*****	1.00	0.00	1800	80	90	20.80	0.000	0.00	0.

RUN NUMBER 360
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
PROPANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.000	0.678	*****	0.75	0.00	1800	115	-	20.80	0.000	0.00	0.
0.029	0.678	97.5	0.75	0.00	1800	38	40	0.82	1.096	10.98	0.
0.031	0.678	90.8	0.75	0.00	1800	39	-	0.74	3.007	9.60	0.
0.035	0.678	79.5	0.75	0.00	1800	41	-	0.71	6.444	7.62	0.
0.038	0.678	73.3	0.75	0.00	1800	36	-	0.69	7.996	6.69	20.
0.041	0.678	67.9	0.75	0.00	1800	13	-	0.67	9.848	5.56	1600.
0.000	0.678	*****	0.75	0.00	1800	95	100	20.80	0.000	0.00	0.
0.000	0.678	*****	0.50	0.00	1800	100	-	20.80	0.000	0.00	0.
0.029	0.678	97.5	0.50	0.00	1800	38	39	0.81	0.983	10.98	0.
0.031	0.678	90.8	0.50	0.00	1800	38	-	0.71	3.104	9.60	0.
0.035	0.678	79.5	0.50	0.00	1800	39	-	0.67	6.287	7.73	0.
0.038	0.678	73.3	0.50	0.00	1800	35	-	0.66	8.186	6.59	30.
0.041	0.678	67.9	0.50	0.00	1800	10	-	0.66	9.626	5.66	2300.
0.000	0.678	*****	0.50	0.00	1800	110	115	20.80	0.000	0.00	0.
0.000	0.678	*****	0.25	0.00	1800	115	115	20.80	0.000	0.00	0.
0.029	0.678	97.5	0.25	0.00	1800	37	39	0.75	0.844	11.23	0.
0.031	0.678	90.8	0.25	0.00	1800	36	-	0.70	3.104	9.60	0.
0.035	0.678	79.5	0.25	0.00	1800	38	-	0.70	6.287	7.73	0.
0.038	0.678	73.3	0.25	0.00	1800	32	-	0.69	8.186	6.69	80.
0.041	0.678	67.9	0.25	0.00	1800	4	-	0.68	9.626	5.77	6700.
0.000	0.678	*****	0.25	0.00	1800	115	120	20.80	0.000	0.00	0.
0.000	0.678	*****	0.05	0.00	1800	120	120	20.80	0.000	0.00	0.
0.029	0.678	97.5	0.05	0.00	1800	35	38	0.75	0.680	11.48	0.

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                               RUN NUMBER  360 CONT
                           ADIABATIC STIRRED COMBUSTOR
                               NORMAL COMBUSTION
                              PROPANE      HOT  WALL

FUEL    AIR     PCT     AXIAL   RADIAL   WALL    NO      NOX     O2      CO      CO2     HC
FLOW    FLOW    STOIC   DIST    DIST     TEMP
(CFM)   (CFM)   AIR     (IN)    (IN)     (C)     (PPM)   (PPM)   (PCT)   (PCT)   (PCT)   (PPM)


0.031   0.678    90.8    0.05    0.00    1800      32      33     0.68   3.007    9.81       0.
0.035   0.678    79.5    0.05    0.00    1800      36       -     0.66   6.134    7.93       0.
0.038   0.678    73.3    0.05    0.00    1800      28       -     0.67   8.186    6.79     260.
0.041   0.678    67.9    0.05    0.00    1800       3       -     0.67   9.626    5.77    7100.
0.000   0.678   *****    0.05    0.00    1800     120     120    20.80   0.000    0.00       0.
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RUN NUMBER 362*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.102	0.708	72.7	3.00	0.00	1600	41	-	0.82	7.448	4.85	5.
0.116	0.708	64.0	3.00	0.00	1600	2	-	0.79	8.985	4.14	2300.
0.130	0.708	57.0	3.00	0.00	1600	0	0	0.79	9.408	3.74	14000.
0.051	0.708	144.3	3.00	0.00	1600	6	8	7.20	0.053	6.69	0.
0.063	0.708	117.0	3.00	0.00	1600	14	16	4.00	0.104	7.83	0.
0.076	0.708	97.8	3.00	0.00	1600	36	38	1.10	1.328	8.46	0.
0.088	0.708	83.5	3.00	0.00	1600	43	-	0.87	4.756	6.28	0.
0.051	0.708	144.3	1.00	0.00	1600	4	5	7.20	0.079	6.59	0.
0.063	0.708	117.0	1.00	0.00	1600	9	11	4.10	0.155	7.73	0.
0.076	0.708	97.8	1.00	0.00	1600	26	29	1.20	1.357	8.25	0.
0.088	0.708	83.5	1.00	0.00	1600	34	-	0.88	4.510	6.48	0.
0.102	0.708	72.7	1.00	0.00	1600	15	-	1.30	7.272	4.95	4000.
0.116	0.708	64.0	1.00	0.00	1600	1	6	2.80	6.287	3.25	46000.
0.130	0.708	57.0	1.00	0.00	1600	0	3	7.70	5.412	2.56	74000.
0.051	0.708	144.3	0.75	0.00	1600	5	7	6.90	0.053	6.59	0.
0.063	0.708	117.0	0.75	0.00	1600	15	18	3.80	0.104	7.93	0.
0.076	0.708	97.8	0.75	0.00	1600	36	38	1.00	1.125	8.56	0.
0.088	0.708	83.5	0.75	0.00	1600	38	-	0.79	4.632	6.59	0.
0.102	0.708	72.7	0.75	0.00	1600	41	-	0.77	7.272	5.05	70.
0.116	0.708	64.0	0.75	0.00	1600	1	-	1.20	8.380	4.14	12000.
0.051	0.708	144.3	0.50	0.00	1600	5	6	7.20	1.877	0.20	5.
0.063	0.708	117.0	0.50	0.00	1600	13	16	3.80	2.302	0.29	0.
0.076	0.708	97.8	0.50	0.00	1600	33	34	1.00	2.541	3.44	0.

* Air leak in sampling system amounting to 4% of sampled volume.

RUN NUMBER 362*CONT
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.088	0.708	83.5	0.50	0.00	1600	36	-	0.77	4.632	6.69	0.
0.102	0.708	72.7	0.50	0.00	1600	38	-	0.75	7.272	5.05	380.
0.116	0.708	64.0	0.50	0.00	1600	0	0	1.20	8.380	4.24	12000.
0.051	0.708	144.3	0.25	0.00	1600	5	7	7.00	0.053	6.79	0.
0.063	0.708	117.0	0.25	0.00	1600	12	15	3.90	0.079	8.04	0.
0.076	0.708	97.8	0.25	0.00	1600	30	32	0.85	0.983	8.77	0.
0.088	0.708	83.5	0.25	0.00	1600	35	-	0.74	4.510	6.79	0.
0.102	0.708	72.7	0.25	0.00	1600	30	-	0.73	7.272	5.15	960.
0.116	0.708	64.0	0.25	0.00	1600	0	0	1.50	8.186	4.04	16000.

* Air leak in sampling system amounting to 4% of sampled volume.

RUN NUMBER 363*
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.051	0.708	144.3	0.05	0.00	1600	6	8	7.30	0.028	6.79	0.
0.063	0.708	117.0	0.05	0.00	1600	9	14	4.10	0.079	8.04	0.
0.076	0.708	97.8	0.05	0.00	1600	25	30	1.30	1.039	8.66	0.
0.088	0.708	83.5	0.05	0.00	1600	41	-	0.86	4.756	6.59	0.
0.102	0.708	72.7	0.05	0.00	1600	33	-	0.69	7.100	5.25	560.
0.116	0.708	64.0	0.05	0.00	1600	1	6	5.70	6.134	3.25	46000.
0.076	0.708	97.8	1.00	0.00	1600	36	38	0.93	0.955	8.66	5.
0.088	0.708	83.5	1.00	0.00	1600	40	-	0.76	4.510	6.59	0.
0.102	0.708	72.7	1.00	0.00	1600	44	-	0.73	7.272	5.05	0.
0.116	0.708	64.0	1.00	0.00	1600	1	-	0.96	8.380	4.14	9500.

* Air leak in sampling system amounting to 4% of sampled volume.

RUN NUMBER 364
PREMIXED FLAT FLAME BURNER
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	PREHEAT TEMP (C)	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.049	0.561	119.9	25.	25.	10.00	0.25	1584	48	54	4.00	0.053	7.93	0.
0.049	0.561	119.9	25.	25.	3.00	0.25	1584	35	39	3.50	0.028	7.73	0.
0.049	0.561	119.9	25.	25.	1.00	0.25	1584	22	25	2.80	0.000	6.07	0.
0.049	0.561	119.9	25.	25.	0.50	0.25	1584	12	15	2.40	0.000	4.85	0.
0.049	0.561	119.9	25.	25.	0.25	0.25	1584	8	10	2.30	0.000	4.55	0.
0.049	0.561	119.9	25.	25.	0.05	0.25	1584	6	9	2.30	0.028	4.44	12.

RUN NUMBER 365
PREMIXED FLAT FLAME BURNER
STAGED COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STOIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NC (PPM)	NOX (PPM)	C2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.116	0.561	5C.8	0.0CC	5C.8	14.7C	0.25	1507	0	0	C.29	11.023	2.66	39CC.
0.116	0.561	5C.8	0.320	79.7	14.7C	0.25	1507	0	0	C.29	11.C23	2.56	4100.
0.116	0.561	50.8	0.32C	79.7	34.3C	C.25	1507	6	0	C.07	5.412	6.69	530.
0.116	0.561	50.8	0.0C0	50.8	34.30	0.25	1507	0	0	C.08	1C.779	2.66	2900.
0.116	0.561	50.8	0.546	100.1	34.3C	0.25	1507	7	8	C.1C	C.440	1C.73	7.
0.116	0.561	5C.8	0.546	100.1	14.70	C.25	1507	0	0	C.25	11.271	2.56	440C.
0.116	0.561	50.8	0.0CC	50.8	14.70	C.25	1507	0	0	C.25	11.023	2.56	400C.

RUN NUMBER 367
PREMIXED FLAT FLAME BURNER
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	PREHEAT TEMP (C)	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.045	0.516	118.7	25.	25.	10.00	0.25	1769	74	83	3.30	0.028	9.81	0.
0.045	0.516	118.7	25.	25.	3.00	0.25	1769	35	41	3.20	0.000	9.71	0.
0.045	0.516	118.7	25.	25.	1.00	0.25	1769	22	25	3.00	0.000	8.77	0.
0.045	0.516	118.7	25.	25.	0.50	0.25	1769	20	23	2.90	0.000	8.46	0.
0.045	0.516	118.7	25.	25.	0.25	0.25	1769	20	22	2.80	0.000	8.35	0.
0.045	0.516	118.7	25.	25.	0.05	0.25	1769	19	22	2.80	0.000	8.25	0.

RUN NUMBER 368
PREMIXED FLAT FLAME BURNER
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	PREHEAT TEMP (C)	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.038	0.516	139.6	25.	25.	10.00	0.25	1584	20	23	5.70	0.000	8.46	0.
0.038	0.516	139.6	25.	25.	3.00	0.25	1584	13	16	5.60	0.000	8.46	0.
0.038	0.516	139.6	25.	25.	1.00	0.25	1584	7	9	5.30	0.000	8.04	0.
0.038	0.516	139.6	25.	25.	0.50	0.25	1584	4	6	5.20	0.000	7.73	0.
0.038	0.516	139.6	25.	25.	0.25	0.25	1584	3	6	5.10	0.000	7.62	0.
0.038	0.516	139.6	25.	25.	0.05	0.25	1584	3	6	5.00	0.028	7.62	2.

RUN NUMBER 369
PREMIXED FLAT FLAME BURNER
STAGED COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STOIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.090	0.516	60.1	0.000	60.1	14.70	0.25	1507	2	3	0.23	10.304	3.54	160.
0.090	0.516	60.1	0.342	100.0	14.70	0.25	1507	2	3	0.24	10.304	3.54	150.
0.090	0.516	60.1	0.342	100.0	34.30	0.25	1507	8	9	0.18	0.440	10.98	0.
0.090	0.516	60.1	0.000	60.1	34.30	0.25	1507	2	3	0.11	9.408	3.74	80.
0.090	0.516	60.1	0.515	120.0	34.30	0.25	1507	7	7	3.70	0.232	8.77	0.
0.090	0.516	60.1	0.515	120.0	14.70	0.25	1507	2	3	0.25	10.304	3.54	200.
0.090	0.516	60.1	0.000	60.1	14.70	0.25	1507	2	3	0.25	10.304	3.54	150.

RUN NUMBER 370
PREMIXED FLAT FLAME BURNER
STAGEC CCMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	PRIMARY AIR FLOW (CFM)	PRIMARY PCT STCIC AIR	SEC. AIR FLOW (CFM)	OVERALL PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NC (PPM)	NCX (PPM)	C2 (PCT)	CO (PCT)	CC2 (PCT)	HC (PPM)
0.068	0.516	79.2	0.000	79.2	14.70	C.25	1821	40	42	C.32	6.765	6.18	0.
0.068	0.516	79.2	0.146	101.7	14.70	C.25	1821	38	39	C.33	6.931	6.07	0.
0.068	0.516	79.2	0.146	101.7	34.30	0.25	1821	26	28	1.90	1.446	8.77	0.
0.068	0.516	79.2	0.000	79.2	34.30	0.25	1821	38	40	1.10	5.412	5.87	0.
0.068	0.516	79.2	0.262	119.6	34.30	C.25	1821	23	25	3.20	0.181	9.08	0.
0.068	0.516	79.2	0.262	119.6	14.70	0.25	1821	41	43	C.38	6.931	5.97	0.
0.068	0.516	79.2	0.000	79.2	14.70	0.25	1821	39	40	C.39	6.765	6.07	0.

RUN NUMBER 371
PREMIXED FLAT FLAME BURNER
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.038	0.516	139.6	170.	10.00	0.25	1712	23	27	6.00	0.000	7.21	0.
0.038	0.516	139.6	170.	3.00	0.25	1712	10	13	5.70	0.000	6.90	0.
0.038	0.516	139.6	170.	1.00	0.25	1712	10	11	5.10	0.000	5.97	0.
0.038	0.516	139.6	170.	0.50	0.25	1712	4	5	4.90	0.000	5.87	0.
0.038	0.516	139.6	170.	0.25	0.25	1712	3	4	4.80	0.000	5.56	0.
0.038	0.516	139.6	170.	0.05	0.25	1712	2	3	4.70	0.028	5.46	15.

RUN NUMBER 372
PREMIXED FLAT FLAME BURNER
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.045	0.516	118.7	170.	10.00	0.25	1883	170	190	3.50	0.079	8.87	0.
0.045	0.516	118.7	170.	3.00	0.25	1883	37	46	3.40	0.028	8.77	0.
0.045	0.516	118.7	170.	1.00	0.25	1883	22	27	3.00	0.000	7.42	0.
0.045	0.516	118.7	170.	0.50	0.25	1883	17	21	2.90	0.000	7.10	0.
0.045	0.516	118.7	170.	0.25	0.25	1883	13	16	2.80	0.000	6.90	0.
0.045	0.516	118.7	170.	0.05	0.25	1883	10	13	2.70	0.000	6.79	0.

RUN NUMBER 374*
PREMIXED FLAT FLAME BURNER
FLUE GAS RECYCLE
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	RECYCLE RATIO	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.053	0.516	100.7	0.00	120.	13.10	0.25	1558	60	62	4.70	0.653	7.93	0.
0.053	0.516	100.7	0.50	120.	13.10	0.25	1558	6	7	5.60	0.000	7.83	0.
0.053	0.516	100.7	0.50	120.	10.00	0.25	1558	5	6	5.70	0.000	7.73	0.
0.053	0.516	100.7	0.50	120.	3.00	0.25	1558	1	3	7.10	0.309	6.59	1500.
0.053	0.516	100.7	0.50	120.	1.00	0.25	1558	2	3	6.50	0.079	7.10	4500.
0.053	0.516	100.7	0.50	120.	0.50	0.25	1558	2	3	10.30	0.000	4.75	27000.
0.053	0.516	100.7	0.50	120.	0.25	0.25	1558	2	3	11.70	0.000	3.74	40000.
0.053	0.516	100.7	0.50	120.	0.05	0.25	1558	2	3	12.10	0.000	3.15	45000.
0.053	0.516	100.7	0.50	120.	13.10	0.25	1558	5	6	5.90	0.000	7.62	5.

* Air leak in sampling system amounting to 20% of sampled volume.

RUN NUMBER 375*
PREMIXED FLAT FLAME BURNER
FLUE GAS RECYCLE
METHANE HCT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	RECYCLE RATIO	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NC (PPM)	NOX (PPM)	C2 (PCT)	CC (PCT)	CC2 (PCT)	HC (PPM)
0.053	0.516	10C.7	0.0C	120.	13.10	C.25	1754	83	84	5.8C	C.789	7.21	C.
0.053	0.516	100.7	0.25	120.	13.1C	C.25	1754	44	48	6.6C	C.053	7.31	C.
0.053	0.516	100.7	0.25	120.	1C.00	C.25	1754	26	29	5.8C	C.104	7.52	C.
0.053	0.516	10C.7	0.25	120.	3.00	0.25	1754	17	19	5.3C	C.C28	7.83	C.
0.053	0.516	100.7	0.25	120.	1.0C	0.25	1754	12	15	5.6C	C.206	7.31	2C.
0.053	0.516	10C.7	0.25	120.	C.50	0.25	1754	11	15	5.7C	C.466	7.31	15C.
0.053	0.516	100.7	0.25	120.	C.25	C.25	1754	5	8	6.8C	C.872	6.48	35CC.
0.053	0.516	100.7	0.25	120.	C.05	0.25	1754	3	4	12.3C	C.028	3.25	42CCC.
0.053	0.516	100.7	0.25	120.	13.10	0.25	1754	40	42	5.7C	C.104	7.52	5.

* Air leak in sampling system amounting to 25% of sampled volume.

RUN NUMBER 376*
PREMIXED FLAT FLAME BURNER
FLUE GAS RECYCLE
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	RECYCLE RATIO	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.053	0.516	100.7	0.00	120.	13.10	0.25	1890	185	190	5.70	1.125	7.10	3.
0.053	0.516	100.7	0.10	120.	13.10	0.25	1890	120	125	5.50	1.211	7.00	0.
0.053	0.516	100.7	0.10	120.	10.00	0.25	1890	58	60	5.90	0.955	7.10	0.
0.053	0.516	100.7	0.10	120.	3.00	0.25	1890	46	47	5.30	0.653	7.42	0.
0.053	0.516	100.7	0.10	120.	1.00	0.25	1890	29	30	5.20	0.546	6.59	0.
0.053	0.516	100.7	0.10	120.	0.50	0.25	1890	37	38	5.70	0.872	7.52	0.
0.053	0.516	100.7	0.10	120.	0.25	0.25	1890	28	31	5.80	1.153	7.62	35.
0.053	0.516	100.7	0.10	120.	0.05	0.25	1890	2	3	12.00	0.899	3.54	40000.
0.053	0.516	100.7	0.10	120.	13.10	0.25	1890	46	48	5.60	1.039	7.00	20.

* Air leak in sampling system amounting to 25% of sampled volume.

RUN NUMBER 377*
PREMIXED FLAT FLAME BURNER
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	BURNER TEMP (C)	AXIAL DIST (IN)	RACIAL DIST (IN)	WALL TEMP (C)	NC (PPM)	NCX (PPM)	C2 (PCT)	CO (PCT)	CC2 (PCT)	HC (PPM)
0.053	0.516	100.7	80.	10.00	0.25	1951	100	105	5.30	1.039	7.10	5.
0.053	0.516	100.7	60.	3.00	0.25	1951	44	46	5.10	0.599	7.21	1.
0.053	0.516	100.7	45.	1.00	0.25	1951	34	35	4.90	0.546	6.28	0.
0.053	0.516	100.7	45.	0.50	0.25	1951	45	46	5.80	0.872	7.21	0.
0.053	0.516	100.7	40.	0.25	0.25	1951	38	41	5.70	1.125	7.62	0.
0.053	0.516	100.7	40.	0.05	0.25	1951	3	4	14.00	0.053	2.08	55000.

* Air leak in sampling system amounting to 25% of sampled volume.

RUN NUMBER 378
PREMIXED FLAT FLAME BURNER
WATER VAPOR ADDITION
METHANE HOT WALL

FUEL FLOW (CFM)	DRY AIR FLOW (CFM)	PCT STOIC AIR	ABS HUMIC (PCT)	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.045	0.516	118.7	0.0	120.	13.10	0.25	1800	170	190	3.00	0.000	8.98	0.
0.045	0.516	118.7	2.0	120.	10.00	0.25	1800	37	53	2.80	0.028	8.87	0.
0.045	0.516	118.7	2.0	120.	3.00	0.25	1800	14	23	2.70	0.000	8.87	0.
0.045	0.516	118.7	2.0	120.	1.00	0.25	1800	16	24	2.10	0.028	7.52	0.
0.045	0.516	118.7	2.0	120.	0.50	0.25	1800	14	23	3.00	0.104	10.73	0.
0.045	0.516	118.7	2.0	120.	0.25	0.25	1800	10	17	3.70	0.104	9.60	0.
0.045	0.516	118.7	2.0	120.	0.05	0.25	1800	1	3	18.00	0.000	0.29	75000.
0.045	0.516	118.7	0.0	120.	13.10	0.25	1800	170	195	3.00	0.028	8.87	5.

RUN NUMBER 379
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	C2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.041	0.516	131.9	10.10	0.00	1725	100	115	4.50	0.079	8.98	0.
0.041	0.516	131.9	3.00	0.00	1725	27	34	4.40	0.104	9.08	1.
0.041	0.516	131.9	1.00	0.00	1725	11	17	4.50	0.181	8.87	0.
0.041	0.516	131.9	0.50	0.00	1725	12	18	4.40	0.155	8.77	1.
0.041	0.516	131.9	0.25	0.00	1725	7	17	4.50	0.309	8.56	350.
0.041	0.516	131.9	0.05	0.00	1725	5	11	5.10	0.493	8.25	1200.
0.041	0.516	131.9	10.10	0.00	1725	90	105	4.50	0.079	9.08	2.

RUN NUMBER 380
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.064	0.516	83.8	10.10	0.00	1824	75	77	0.18	6.287	6.90	0.
0.064	0.516	83.8	3.00	0.00	1824	62	63	0.19	5.984	7.10	0.
0.064	0.516	83.8	1.00	0.00	1824	44	47	0.18	5.693	7.42	90.
0.064	0.516	83.8	0.50	0.00	1824	26	30	0.53	5.551	7.21	3000.
0.064	0.516	83.8	0.25	0.00	1824	25	39	0.75	5.412	7.00	4200.
0.064	0.516	83.8	0.05	0.00	1824	13	32	2.00	5.551	6.48	9500.
0.064	0.516	83.8	10.10	0.00	1824	67	69	0.19	6.287	7.00	7.

RUN NUMBER 381
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.051	0.516	105.3	10.10	0.00	1953	850	860	0.58	1.096	10.73	3.
0.051	0.516	105.3	3.00	0.00	1953	105	115	0.58	1.211	10.98	0.
0.051	0.516	105.3	1.00	0.00	1953	36	45	0.72	1.182	10.73	1.
0.051	0.516	105.3	0.50	0.00	1953	28	37	0.73	1.153	10.73	35.
0.051	0.516	105.3	0.25	0.00	1953	28	35	1.00	1.096	10.49	1000.
0.051	0.516	105.3	0.05	0.00	1953	16	28	2.60	1.973	8.66	6500.
0.051	0.516	105.3	10.10	0.00	1953	760	780	0.54	1.182	10.98	5.

RUN NUMBER 382
ADIABATIC STIRRED COMBUSTCR
NORMAL CCMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NC (PPM)	NOX (PPM)	C2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.025	0.248	101.3	10.10	0.00	1953	1300	135C	0.60	0.983	10.98	1.
0.025	0.248	101.3	3.00	0.00	1953	100	110	C.58	0.519	11.48	0.
0.025	0.248	101.3	1.00	0.0C	1953	45	51	C.67	0.599	11.48	0.
0.025	0.248	1C1.3	0.50	0.0C	1953	36	42	C.70	0.573	11.23	1.
0.025	0.248	101.3	0.25	0.00	1953	37	42	C.65	0.519	11.48	0.
0.025	0.248	101.3	0.05	0.0C	1953	35	41	1.20	1.153	10.73	7.
0.025	C.248	101.3	10.10	0.0C	1953	1250	130C	C.66	0.872	10.98	2.

RUN NUMBER 383
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.051	0.492	100.3	10.10	0.00	1953	760	780	0.56	1.153	10.98	3.
0.051	0.492	100.3	0.25	0.00	1953	39	48	0.97	1.328	10.73	0.
0.045	0.492	113.0	0.25	0.00	1953	21	30	2.90	0.466	9.92	0.
0.040	0.492	129.1	0.25	0.00	1953	14	21	5.20	0.258	8.87	1.
0.057	0.492	89.9	0.25	0.00	1953	55	58	0.27	3.506	9.29	5.
0.063	0.492	81.3	0.25	0.00	1953	54	57	0.19	5.551	7.73	80.
0.069	0.492	74.1	0.25	0.00	1953	42	51	0.25	7.272	6.59	1700
0.055	0.492	93.8	0.25	0.00	1953	49	52	0.39	2.632	9.71	5.

RUN NUMBER 384
ADIABATIC STIRRED COMBUSTOR
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	C2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.021	0.248	121.1	150.	10.10	0.00	1800	440	490	4.50	0.129	9.29	0.
0.021	0.248	121.1	150.	3.00	0.00	1800	44	58	4.60	0.053	9.39	0.
0.021	0.248	121.1	150.	1.00	0.00	1800	26	36	4.60	0.079	9.39	0.
0.021	0.248	121.1	150.	0.50	0.00	1800	21	29	4.60	0.079	9.29	0.
0.021	0.248	121.1	150.	0.25	0.00	1800	20	27	4.70	0.129	9.29	1.
0.021	0.248	121.1	150.	0.05	0.00	1800	15	24	4.80	0.414	9.08	1.

RUN NUMBER 385
ADIABATIC STIRRED COMBUSTOR
PREHEATED AIR
METHANE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	BURNER TEMP (C)	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.041	0.492	125.6	150.	10.10	0.00	1800	220	245	4.40	0.129	9.29	1.
0.041	0.492	125.6	150.	3.00	0.00	1800	40	52	4.30	0.079	9.50	0.
0.041	0.492	125.6	150.	1.00	0.00	1800	21	29	4.40	0.155	9.50	0.
0.041	0.492	125.6	150.	0.50	0.00	1800	16	24	4.40	0.206	9.39	0.
0.041	0.492	125.6	150.	0.25	0.00	1800	12	21	4.50	0.283	9.29	1.
0.041	0.492	125.6	150.	0.05	0.00	1800	10	18	4.80	0.762	8.77	1.

RUN NUMBER 386
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
HYDROGEN HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.346	0.492	59.7	10.10	0.00	1910	16	1	0.24	0.000	0.00	0.
0.346	0.492	59.7	3.00	0.00	1910	6	1	0.23	0.000	0.00	0.
0.346	0.492	59.7	1.00	0.00	1910	5	1	0.23	0.000	0.00	0.
0.346	0.492	59.7	0.50	0.00	1910	5	1	0.22	0.000	0.00	0.
0.346	0.492	59.7	0.25	0.00	1910	4	1	0.22	0.000	0.00	0.
0.346	0.492	59.7	0.05	0.00	1910	4	1	0.45	0.000	0.00	0.

RUN NUMBER 387
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
HYDROGEN HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.172	0.492	130.0	10.10	0.00	1897	620	680	4.70	0.000	0.00	0.
0.172	0.492	130.0	3.00	0.00	1897	34	44	4.80	0.000	0.00	0.
0.172	0.492	130.0	1.00	0.00	1897	13	18	4.70	0.000	0.00	0.
0.172	0.492	130.0	0.50	0.00	1897	10	14	4.60	0.000	0.00	0.
0.172	0.492	130.0	0.25	0.00	1897	8	11	4.70	0.000	0.00	0.
0.172	0.492	130.0	0.05	0.00	1897	7	10	5.00	0.000	0.00	0.

RUN NUMBER 388
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
HYDROGEN HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.089	0.248	127.0	10.10	0.00	1897	1150	1250	4.30	0.000	0.00	0.
0.089	0.248	127.0	3.00	0.00	1897	36	51	4.80	0.000	0.00	0.
0.089	0.248	127.0	1.00	0.00	1897	13	20	4.70	0.000	0.00	0.
0.089	0.248	127.0	0.50	0.00	1897	9	14	4.50	0.000	0.00	0.
0.089	0.248	127.0	0.25	0.00	1897	8	12	4.50	0.000	0.00	0.
0.089	0.248	127.0	0.05	0.00	1897	8	11	5.30	0.000	0.00	0.

RUN NUMBER 389
ADIABATIC STIRRED COMBUSTOR
NORMAL COMBUSTION
HYDROGEN HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	C2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.159	0.492	150.7	10.10	0.00	1685	33	45	7.20	0.000	0.00	0.
0.159	0.492	150.7	3.00	0.00	1685	11	17	7.20	0.000	0.00	0.
0.159	0.492	150.7	1.00	0.00	1685	7	10	7.00	0.000	0.00	0.
0.159	0.492	150.7	0.50	0.00	1685	6	9	6.90	0.000	0.00	0.
0.159	0.492	150.7	0.25	0.00	1685	5	8	6.80	0.000	0.00	0.
0.159	0.492	150.7	0.05	0.00	1685	5	7	7.10	0.000	0.00	0.

RUN NUMBER 390
ADIABATIC STIRRED COMBUSTOR
H2 ADDITION
CARBON MONOXIDE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR (CO)	ADDITIVE FLOW (H2)	OVERALL STOICH AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.133	0.516	163.0	0.023	139.0	10.10	0.00	1736	900	950	6.80	0.335		
0.133	0.516	163.0	0.023	139.0	3.00	0.00	1736	135	160	6.50	0.232	*****	0.
0.133	0.516	163.0	0.023	139.0	1.00	0.00	1736	38	45	6.20	0.079	*****	0.
0.133	0.516	163.0	0.023	139.0	0.50	0.00	1736	20	27	6.30	0.388	*****	0.
0.133	0.516	163.0	0.023	139.0	0.25	0.00	1736	12	19	6.50	0.816	*****	0.
0.133	0.516	163.0	0.023	139.0	0.05	0.00	1736	10	17	6.70	1.417	24.72	1.

RUN NUMBER 391
ADIABATIC STIRRED COMBUSTOR
H2 ADDITION
CARBON MONOXIDE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR (CO)	ADDITIVE FLOW (H2)	OVERALL STOICH AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.151	0.516	143.6	0.023	124.6	10.10	0.00	1877	880	930	5.10	0.493	*****	0.
0.151	0.516	143.6	0.023	124.6	3.00	0.00	1877	155	175	5.20	0.546	*****	0.
0.151	0.516	143.6	0.023	124.6	1.00	0.00	1877	38	50	5.00	0.388	*****	0.
0.151	0.516	143.6	0.023	124.6	0.50	0.00	1877	23	33	5.20	0.707	*****	0.
0.151	0.516	143.6	0.023	124.6	0.25	0.00	1877	16	25	5.40	1.211	*****	0.
0.151	0.516	143.6	0.023	124.6	0.05	0.00	1877	13	21	5.60	1.845	*****	0.

RUN NUMBER 392
ADIABATIC STIRRED COMBUSTOR
H2 ADDITION
CARBON MONOXIDE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR (CO)	ADDITIVE FLOW (CFM) (H2)	OVERALL STOICH AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.429	0.516	50.6	0.023	48.0	10.10	0.00	1877	44	46	0.11	******	*****	0.
0.429	0.516	50.6	0.023	48.0	3.00	0.00	1877	30	31	0.11	******	*****	0.
0.429	0.516	50.6	0.023	48.0	1.00	0.00	1877	17	19	0.10	******	*****	0.
0.429	0.516	50.6	0.023	48.0	0.50	0.00	1877	12	14	0.10	******	*****	0.
0.429	0.516	50.6	0.023	48.0	0.25	0.00	1877	14	15	0.12	******	*****	0.
0.429	0.516	50.6	0.023	48.0	0.05	0.00	1877	12	14	0.14	******	*****	0.

RUN NUMBER 393
ADIABATIC STIRRED COMBUSTOR
H2 ADDITION
CARBON MONOXIDE HOT WALL

FUEL FLOW (CFM)	AIR FLOW (CFM)	PCT STOIC AIR (CO)	ADDITIVE FLOW (CFM) (H2)	OVERALL STOICH AIR	AXIAL DIST (IN)	RADIAL DIST (IN)	WALL TEMP (C)	NO (PPM)	NOX (PPM)	O2 (PCT)	CO (PCT)	CO2 (PCT)	HC (PPM)
0.429	0.516	50.6	0.000	50.6	10.10	0.00	1877	240	245	0.19	******	*****	0.
0.429	0.516	50.6	0.000	50.6	3.00	0.00	1877	155	160	0.19	******	*****	0.
0.429	0.516	50.6	0.000	50.6	1.00	0.00	1877	42	43	0.19	******	*****	0.
0.429	0.516	50.6	0.000	50.6	0.50	0.00	1877	27	27	0.19	******	*****	0.
0.429	0.516	50.6	0.000	50.6	0.25	0.00	1877	16	17	0.19	******	*****	0.
0.429	0.516	50.6	0.000	50.6	0.05	0.00	1877	8	11	3.50	******	*****	0.

APPENDIX B

EVALUATION OF PROBABLE RELATIVE IMPORTANCE OF REACTION STEPS FOR METHANE/AIR COMBUSTION

This section contains a reaction-by-reaction evaluation of the potential importance of each of the 322 reactions considered in this study. It is extremely important to understand the groundrules for the evaluation and scope of its applicability. The comments found in this section refer only to the combustion of methane-air from 80-125% stoichiometric air, from 1500-2500K. This has been stated elsewhere in this report, but bears repeating. The use of the information in this section outside the limits mentioned, may be valid, but should be approached with caution. Not only would the relative importance of the given reactions require evaluation for specific conditions but other species and, therefore, additional reactions might have to be considered outside those limits. And of course, other reaction systems such as higher hydrocarbons of fuel-nitrogen containing systems would bear their own evaluations.

The headings in this section are as follows:

Headings	Description
REACTION	Written in both directions Reaction number indicated F = Forward R = Reverse
HR	ΔH_r for both directions given at 2000K (mid-range of 1500-2500K) note: in the thermochemical tables ΔH_{r298} is used in the expression for log K_c
NOTES	A Probably important B Possibly important C Probably unimportant * Flag indicating reaction was rated either A or B
COMMENTS	Notes explaining reasons for ranking

REACTION	HR	NOTES	COMMENTS
1F. CH + CHN = CH2 + CN 1R. CH2 + CN = CH + CHN	20.3 -20.3	B * B *	CONSIDER BOTH DIRECTIONS, FUEL RICH POSSIBLE ROLE CN/HCN PROBABLY MINOR
2F. CH + CHO = CH2 + CO 2R. CH2 + CO = CH + CHO	-85.5 85.5	C C	FORWARD UNIMPORTANT FOR CHO REMOVAL H, O, HO MORE LIKELY REACTION PARTNERS REVERSE ENDOTHERMIC
3F. CH + CH2O = CHO + CH2 3R. CHO + CH2 = CH + CH2O	-15.6 15.6	C C	CH, CH2 MINOR RX PARTNERS FOR CHO, CH2O
4F. CH + CH2O = CH3 + CO 4R. CH3 + CO = CH + CH2O	-108.6 108.6	C C	CH MINOR RX PARTNER FOR CH2O REVERSE HIGHLY ENDOTHERMIC
5F. CH + CH3 = CH2 + CH2 5R. CH2 + CH2 = CH + CH3	7.4 -7.4	C C	(CH)(CH3) AND (CH2)(CH2) LIKELY SMALL POSSIBLE FUEL RICH
6F. CH + CH3O = CHO + CH3 6R. CHO + CH3 = CH + CH3O	-102.7 102.7	C C	LOW CONCENTRATIONS FORWARD REVERSE HIGHLY ENDOTHERMIC
7F. CH + CH3O = CH2 + CH2O 7R. CH2 + CH2O = CH + CH3O	-79.6 79.6	C C	LOW CONCENTRATIONS FORWARD REVERSE ENDOTHERMIC
8F. CH + CH3O = CH4 + CO 8R. CH4 + CO = CH + CH3O	-191.3 191.3	C C	NOT LIKELY TO BE ELEMENTARY REACTION
9F. CH + CH4 = CH2 + CH3 9R. CH2 + CH3 = CH + CH4	3.0 -3.0	B * B *	CONSIDER BOTH DIRECTIONS, FUEL RICH CH4 STARTING MATL, CH3 INITIAL INTERMED THERMALLY NEUTRAL
10F. CH + CO2 = CHO + CO 10R. CHO + CO = CH + CO2	-68.3 68.3	B * C	CONSIDER FORWARD, FUEL RICH (CO2) HIGH, PATH FROM CH TO CO REVERSE ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
11F. CH + H + M = CH2 + M	-105.1	C	THIRD ORDER, LOW CONC IN FORWARD
11R. CH2 + M = CH + H + M	105.1	C	REVERSE HIGHLY ENDOTHERMIC
12F. CH + HN = CHN + H	-145.4	C	LOW CONCENTRATIONS FORWARD
12R. CHN + H = CH + HN	145.4	C	HIGHLY ENDOTHERMIC REVERSE
13F. CH + HN = CH2 + N	-26.2	C	LOW CONCENTRATIONS BOTH DIRECTIONS
13R. CH2 + N = CH + HN	26.2	C	
14F. CH + HN = CN + H2	-128.4	C	LOW CONCENTRATIONS FORWARD
14R. CN + H2 = CH + HN	128.4	C	REVERSE HIGHLY ENDOTHERMIC
			FOUR-CENTER REACTION
15F. CH + HNO = CHN + HO	-123.8	C	FORWARD POSSIBLE FOR NOH STRUCTURE
15R. CHN + HO = CH + HNO	123.8	C	CONCENTRATIONS LOW
			REVERSE HIGHLY ENDOTHERMIC
16F. CH + HNO = CHO + HN	-67.8	C	LOW CONCENTRATIONS BOTH DIRECTIONS
16R. CHO + HN = CH + HNO	67.8	C	REVERSE ENDOTHERMIC
17F. CH + HNO = CH2 + NO	-52.4	C	LOW CONCENTRATIONS FORWARD
17R. CH2 + NO = CH + HNO	52.4	C	CH2 + NO = CH2O + N MORE LIKELY REVERSE
18F. CH + HNO = CH2O + N	-78.4	C	LOW CONCENTRATIONS FORWARD
18R. CH2O + N = CH + HNO	78.4	C	REVERSE ENDOTHERMIC
19F. CH + HNO = CN + H2O	-121.7	C	LOW CONCENTRATIONS FORWARD
19R. CN + H2O = CH + HNO	121.7	C	REVERSE HIGHLY ENDOTHERMIC
			FOUR-CENTER REACTION FOR NOH STRUCTURE
20F. CH + HO = CHO + H	-89.4	B *	CONSIDER FORWARD
20R. CHO + H = CH + HO	89.4	C	REVERSE ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
21F. CH + HO = CH2 + O	1.2	C	CH + HO = CHO + H MORE LIKELY FORWARD
21R. CH2 + O = CH + HO	-1.2	C	CH2 + O = CHO + H MORE LIKELY REVERSE
22F. CH + HO + M = CH2O + M	-178.9	C	THIRD ORDER, LOW CONCENTRATION FORWARD
22R. CH2O + M = CH + HO + M	178.9	C	REVERSE HIGHLY ENDOTHERMIC NOT LIKELY TO BE ELEMENTARY REACTION
23F. CH + HO = CO + H2	-178.3	C	FOUR-CENTER REACTION
23R. CO + H2 = CH + HO	178.3	C	CH + HO = CHO + H MORE LIKELY FORWARD REVERSE HIGHLY ENDOTHERMIC
24F. CH + HO2 = CHO + HO	-129.6	C	H-O2 WEAKER THAN HO-O
24R. CHO + HO = CH + HO2	129.6	C	CH + HO2 = CH2 + HO2 MORE LIKELY FORWARD REVERSE HIGHLY ENDOTHERMIC
25F. CH + HO2 = CH2+ O2	-54.7	B *	CONSIDER FORWARD
25R. CH2+ O2 = CH + HO2	54.7	C	REVERSE ENDOTHERMIC
26F. CH + HO2 = CH2O + O	-112.8	C	NOT LIKELY TO BE ELEMENTARY REACTION
26R. CH2O + O = CH + HO2	112.8	C	
27F. CH + HO2 = CO + H2O	-233.4	C	FOUR-CENTER REACTION
27R. CO + H2O = CH + HO2	233.4	C	CH + HO2 = CH2 + O2 MORE LIKELY FORWARD REVERSE HIGHLY ENDOTHERMIC
28F. CH + HO2 = CO2 + H2	-239.7	C	NOT LIKELY TO BE ELEMENTARY REACTION
28R. CO2 + H2 = CH + HO2	239.7	C	
29F. CH + H2 = CH2 + H	3.4	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
29R. CH2 + H = CH + H2	-3.4	B *	
30F. CH + H2 + M = CH3 + M	-109.2	C	NOT LIKELY TO BE ELEMENTARY REACTION
30R. CH3 + M = CH + H2 + M	109.2	C	

REACTION	HR	NOTES	COMMENTS
31F. CH + H2O = CHO + H2	-74.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
31R. CHO + H2 = CH + H2O	74.5	C	
32F. CH + H2O = CH2+ HO	18.2	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
32R. CH2+ HO = CH + H2O	-18.2	B *	
33F. CH + H2O = CH2O + H	-55.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
33R. CH2O + H = CH + H2O	55.6	C	
34F. CH + H2O = CH3 + O	12.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
34R. CH3 + O = CH + H2O	-12.0	C	
35F. CH + H2O + M = CH3O + M	-81.1	C	NOT LIKELY TO BE ELEMENTARY REACTION
35R. CH3O + M = CH + H2O + M	81.1	C	
36F. CH + N + M = CHN + M	-224.3	C	THIRD ORDER, LOW CONCENTRATIONS FORWARD
36R. CHN + M = CH + N + M	224.3	C	REVERSE HIGHLY ENDOTHERMIC
37F. CH + N = CN + H	-98.9	C	LOW CONCENTRATIONS FORWARD
37R. CN + H = CH + N	98.9	C	REVERSE HIGHLY ENDOTHERMIC
38F. CH + NO = CHN + O	-70.2	B *	CONSIDER FORWARD FUEL RICH
38R. CHN + O = CH + NO	70.2	C	REVERSE ENDOTHERMIC
39F. CH + NO = CHO + N	-41.6	B *	CONSIDER FORWARD FUEL RICH
39R. CHO + N = CH + NO	41.6	C	REVERSE ENDOTHERMIC
40F. CH + NO = CN + HO	-51.1	C	FOUR-CENTER REACTION
40R. CN + HO = CH + NO	51.1	C	

REACTION	HR	NOTES	COMMENTS
41F. CH + NO = CO + HN	-101.0	C	FOUR-CENTER REACTION
41R. CO + HN = CH + NO	101.0	C	
42F. CH + NO2 = CHN + O2	-117.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
42R. CHN + O2 = CH + NO2	117.5	C	
43F. CH + NO2 = CHO + NO	-121.0	C	LOW CONCENTRATIONS FORWARD
43R. CHO + NO = CH + NO2	121.0	C	REVERSE HIGHLY ENDOTHERMIC
44F. CH + NO2 = CN + HO2	-42.4	C	NOT LIKELY TO BE ELEMENTARY REACTION
44R. CN + HO2 = CH + NO2	42.4	C	
45F. CH + NO2 = CO + HNO	-154.1	C	LOW CONCENTRATIONS FORWARD
45R. CO + HNO = CH + NO2	154.1	C	REVERSE HIGHLY ENDOTHERMIC
46F. CH + NO2 = CO2 + HN	-153.7	C	NOT LIKELY TO BE ELEMENTARY REACTION
46R. CO2 + HN = CH + NO2	153.7	C	
47F. CH + N2 = CHN + N	5.1	A *	FORWARD IS LOW ENERGY N-N BREAKING
47R. CHN + N = CH + N2	-5.1	B *	POTENTIALY VERY IMPORTANT
			SPIN RETARDED
			CONSIDER BOTH DIRECTIONS
48F. CH + N2 = CN + HN	51.6	B *	FOUR-CENTER REACTION
48R. CN + HN = CH + N2	-51.6	B *	FORWARD IS MODERATE ENERGY N-N BREAKING
			CONSIDER BOTH DIRECTIONS FOR SCREENING
49F. CH + N2O = CHN + NO	-109.1	C	LOW CONCENTRATIONS FORWARD
49R. CHN + NO = CH + N2O	109.1	C	REVERSE HIGHLY ENDOTHERMIC
50F. CH + N2O = CHO + N2	-155.8	C	LOW CONCENTRATIONS FORWARD
50R. CHO + N2 = CH + N2O	155.8	C	REVERSE HIGHLY ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
51F. CH + N2O = CN + HNO	-36.4	C	LOW CONCENTRATIONS BOTH DIRECTIONS
51R. CN + HNO = CH + N2O	36.4	C	
52F. CH + O + M = CHO + M	-195.7	C	THIRD ORDER, LOW CONCENTRATIONS FORWARD
52R. CHO + M = CH + O + M	195.7	C	REVERSE HIGHLY ENDOTHERMIC
53F. CH + O = CO + H	-176.2	B *	CONSIDER FORWARD
53R. CO + H = CH + O	176.2	C	REVERSE HIGHLY ENDOTHERMIC
54F. CH + O2 = CHO + O	-73.7	B *	CONSIDER FORWARD
54R. CHO + O = CH + O2	73.7	C	REVERSE ENDOTHERMIC
55F. CH + O2 = CO + HO	-160.4	C	FOUR-CENTER REACTION
55R. CO + HO = CH + O2	160.4	C	CH + O2 = CHO + O MORE LIKELY FORWARD
			REVERSE HIGHLY ENDOTHERMIC
56F. CH + O2 = CO2 + H	-181.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
56R. CO2 + H = CH + O2	181.6	C	
57F. CHN + M = CN + H + M	125.4	C	FORWARD HIGHLY ENDOTHERMIC
57R. CN + H + M = CHN + M	-125.4	C	THIRD ORDER, LOW CONCENTRATIONS REVERSE
58F. CHN + CHO = CH2O + CN	35.9	C	LOW CONCENTRATIONS, STERIC HINDRANCE
58R. CH2O + CN = CHN + CHO	-35.9	C	
59F. CHN + CH2 = CH3 + CN	12.9	B *	CONSIDER FUEL RICH
59R. CH3 + CN = CHN + CH2	-12.9	B *	REVERSE POSSIBLE DURING EARLY STAGES
60F. CHN + CH2O = CH3O + CN	99.9	C	STERIC HINDRANCE, LOW CONCENTRATIONS
60R. CH3O + CN = CHN + CH2O	-99.9	C	BOTH DIRECTIONS

REACTION	HR	NOTES	COMMENTS
61F. $CHN + CH_3 = CH_4 + CN$	17.3	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
61R. $CH_4 + CN = CHN + CH_3$	-17.3	B *	REVERSE POSSIBLE DURING EARLY STAGES
62F. $CHN + CO = CHO + CN$	105.9	C	FORWARD HIGHLY ENDOTHERMIC
62R. $CHO + CN = CHN + CO$	-105.9	C	LOW CONCENTRATIONS REVERSE
63F. $CHN + H = CH_2 + N$	119.2	C	FORWARD HIGHLY ENDOTHERMIC
63R. $CH_2 + N = CHN + H$	-119.2	C	LOW CONCENTRATIONS REVERSE
64F. $CHN + H = CN + H_2$	17.0	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
64R. $CN + H_2 = CHN + H$	-17.0	B *	
65F. $CHN + HN = CH_2 + N_2$	-31.3	C	LOW CONCENTRATIONS FORWARD
65R. $CH_2 + N_2 = CHN + HN$	31.3	B *	CONSIDER REVERSE FOR N-N BREAKING FOUR-CENTER REACTION
66F. $CHN + HNO = CH_2 + N_2O$	56.8	C	LOW CONCENTRATIONS BOTH DIRECTIONS
66R. $CH_2 + N_2O = CHN + HNO$	-56.8	C	FOUR-CENTER REACTION
67F. $CHN + HNO = CH_2O + N_2$	-83.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
67R. $CH_2O + N_2 = CHN + HNO$	83.5	C	
68F. $CHN + HO = CHO + HN$	56.0	C	FOUR-CENTER REACTION
68R. $CHO + HN = CHN + HO$	-56.0	C	FORWARD ENDOTHERMIC LOW CONCENTRATIONS REVERSE
69F. $CHN + HO = CH_2 + NO$	71.4	C	FOUR-CENTER REACTION
69R. $CH_2 + NO = CHN + HO$	-71.4	C	FORWARD ENDOTHERMIC $CH_2 + NO = CH_2O + N$ MORE LIKELY REVERSE
70F. $CHN + HO = CH_2O + N$	45.4	C	NOT LIKELY TO BE ELEMENTARY REACTION
70R. $CH_2O + N = CHN + HO$	-45.4	C	

REACTION	HR	NOTES	COMMENTS
71F. CHN + HO = CN + H2O	2.1	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
71R. CN + H2O = CHN + HO	-2.1	B *	
72F. CHN + HO2 = CHO + HNO	-5.8	C	UNLIKELY TO BE ELEMENTARY REACTION
72R. CHO + HNO = CHN + HO2	5.8	C	FOUR-CENTER REACTION STERIC HINDRANCE
73F. CHN + HO2 = CH2 + NO2	62.8	C	FOUR-CENTER REACTION
73R. CH2 + NO2 = CHN + HO2	-62.8	C	FORWARD ENDOTHERMIC LOW CONCENTRATIONS REVERSE
74F. CHN + HO2 = CH2O + NO	-42.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
74R. CH2O + NO = CHN + HO2	42.6	C	
75F. CHN + H2 = CH2 + HN	148.8	C	FOUR-CENTER REACTION
75R. CH2 + HN = CHN + H2	-148.8	C	C-N BOND STRONG REVERSE HIGHLY ENDOTHERMIC
76F. CHN + H2 = CH3 + HN	115.1	C	NOT LIKELY TO BE ELEMENTARY REACTION
76R. CH3 + HN = CHN + H2	-115.1	C	
77F. CHN + H2O = CH2 + HNO	142.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
77R. CH2 + HNO = CHN + H2O	-142.0	C	STERIC HINDRANCE
78F. CHN + H2O = CH2O + HN	89.8	C	NOT LIKELY TO BE ELEMENTARY REACTION
78R. CH2O + HN = CHN + H2O	-89.8	C	
79F. CHN + H2O = CH3 + NO	82.2	C	NOT LIKELY TO BE ELEMENTARY REACTION
79R. CH3 + NO = CHN + H2O	-82.2	C	
80F. CHN + H2O = CH3O + N	143.3	C	NOT LIKELY TO BE ELEMENTARY REACTION
80R. CH3O + N = CHN + H2O	-143.3	C	

REACTION	HR	NOTES	COMMENTS
81F. CHN + N = CN + HN	46.5	C	LOW CONCENTRATIONS BOTH DIRECTIONS
81R. CN + HN = CHN + N	-46.5	C	
82F. CHN + NO = CHO + N2	-46.7	C	FOUR-CENTER REACTION LOW CONCENTRATIONS FORWARD REVERSE ENDOTHERMIC
82R. CHO + N2 = CHN + NO	46.7	C	
83F. CHN + NO = CN + HNO	72.7	C	FORWARD ENDOTHERMIC LOW CONCENTRATIONS REVERSE
83R. CN + HNO = CHN + NO	-72.7	C	
84F. CHN + NO2 = CHO + N2O	-11.8	C	FOUR-CENTER REACTION STERIC HINDRANCE
84R. CHO + N2O = CHN + NO2	11.8	C	
85F. CHN + O = CHO + N	28.6	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
85R. CHO + N = CHN + O	-28.6	B *	
86F. CHN + O = CN + HO	19.1	B *	CONSIDER BOTH DIRECTIONS FUEL RICH NOTE- CNO POSSIBLE PRODUCT REVERSE
86R. CN + HO = CHN + O	-19.1	B *	
87F. CHN + O = CO + HN	-30.8	C	NOT LIKELY TO BE ELEMENTARY REACTION
87R. CO + HN = CHN + O	30.8	C	
88F. CHN + O2 = CHO + NO	-3.4	C	FOUR-CENTER REACTION CHN AND O2 NOT LIKELY HI SIMULTANEOUSLY
88R. CHO + NO = CHN + O2	3.4	C	
89F. CHN + O2 = CN + HO2	75.1	C	FORWARD ENDOTHERMIC LOW CONCENTRATIONS REVERSE
89R. CN + HO2 = CHN + O2	-75.1	C	
90F. CHN + O2 = CO + HNO	-36.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
90R. CO + HNO = CHN + O2	36.6	C	

REACTION	HR	NOTES	COMMENTS
91F. CHN + O2 = CO2 + HN	-36.2	C	NOT LIKELY TO BE ELEMENTARY REACTION
91R. CO2 + HN = CHN + O2	36.2	C	
92F. CHO + M = CO + H + M	19.6	A *	WEAK BOND FORWARD
92R. CO + H + M = CHO + M	-19.6	C	THIRD ORDER REVERSE
93F. CHO + CHO = CH2 + CO2	-17.3	C	FOUR-CENTER REACTION
93R. CH2 + CO2 = CHO + CHO	17.3	C	STERIC HINDRANCE
94F. CHO + CHO = CH2O + CO	-69.9	B *	WEAK BOND FORWARD
94R. CH2O + CO = CHO + CHO	69.9	C	REVERSE ENDOTHERMIC
95F. CHO + CH2 = CH3 + CO	-93.0	B *	WEAK BOND FORWARD
95R. CH3 + CO = CHO + CH2	93.0	C	REVERSE ENDOTHERMIC
96F. CHO + CH2O = CH3 + CO2	-40.3	C	NOT LIKELY TO BE ELEMENTARY REACTION
96R. CH3 + CO2 = CHO + CH2O	40.3	C	
97F. CHO + CH2O = CH3O + CO	-5.9	C	LARGE MOLECULES, LOW CONCENTRATIONS
97R. CH3O + CO = CHO + CH2O	5.9	C	LIKELY TO BE UNIMPORTANT
98F. CHO + CH3 = CH2 + CH2O	23.0	B *	RETAIN FORWARD FOR COMPARISON WITH
98R. CH2 + CH2O = CHO + CH3	-23.0	C	CHO + CH3 = CH4 + CO LOW CONCENTRATIONS REVERSE
99F. CHO + CH3 = CH4 + CO	-88.6	B *	WEAK BOND FORWARD
99R. CH4 + CO = CHO + CH3	88.6	C	REVERSE ENDOTHERMIC
100F. CHO + CH3O = CH2O + CH2O	-64.0	C	LARGE MOLECULES, LOW CONCENTRATIONS
100R. CH2O + CH2O = CHO + CH3O	64.0	C	LIKELY TO BE SLOW

REACTION	HR	NOTES	COMMENTS
101F. CHO + CH3O = CH4 + CO2	-123.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
101R. CH4 + CO2 = CHO + CH3O	123.0	C	
102F. CHO + CH4 = CH2 + CH3O	105.7	C	NOT LIKELY TO BE ELEMENTARY REACTION
102R. CH2 + CH3O = CHO + CH4	-105.7	C	
103F. CHO + CH4 = CH2O + CH3	18.6	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
103R. CH2O + CH3 = CHO + CH4	-18.6	B *	
104F. CHO + H = CH2 + O	90.6	C	FORWARD ENDOTHERMIC
104R. CH2 + O = CHO + H	-90.6	B *	CONSIDER REVERSE
105F. CHO + H + M = CH2O + M	-89.5	C	THIRD ORDER FORWARD
105R. CH2O + M = CHO + H + M	89.5	C	REVERSE ENDOTHERMIC
106F. CHO + H = CO + H2	-88.9	A *	CONSIDER FORWARD FOR CHO BREAKDOWN
106R. CO + H2 = CHO + H	88.9	C	REVERSE ENDOTHERMIC
107F. CHO + HN = CH2 + NO	15.4	C	FOUR-CENTER REACTION
107R. CH2 + NO = CHO + HN	-15.4	C	LOW CONCENTRATIONS BOTH DIRECTIONS
108F. CHO + HN = CH2O + N	-10.6	C	LOW CONCENTRATIONS BOTH DIRECTIONS
108R. CH2O + N = CHO + HN	10.6	C	
109F. CHO + HN = CN + H2O	-53.9	C	NOT LIKELY TO BE ELEMENTARY REACTION
109R. CN + H2O = CHO + HN	53.9	C	
110F. CHO + HNO = CH2 + NO2	68.6	C	FOUR-CENTER REACTION
110R. CH2 + NO2 = CHO + HNO	-68.6	C	ENDOTHERMIC FORWARD
			LOW CONCENTRATIONS REVERSEHO AND CH2O

REACTION	HR	NOTES	COMMENTS
111F. CHO + HNO = CH2O + NO	-36.8	C	UNIMPORTANT PATH BETWEEN CHO AND CH2O
111R. CH2O + NO = CHO + HNO	36.8	C	BETWEEN HNO AND NO
112F. CHO + HO = CH2 + O2	74.9	C	FOUR CENTER REACTION
112R. CH2 + O2 = CHO + HO	-74.9	C	CHO + HO = CO + H2O FASTER THAN FORWARD
			CH2 + O2 = CH2O + O FASTER THAN REVERSE
113F. CHO + HO = CH2O + O	16.8	C	CHO + HO = CO + H2O FASTER THAN FORWARD
113R. CH2O + O = CHO + HO	-16.8	A *	CONSIDER REVERSE FOR CH2O BREAKDOWN
114F. CHO + HO = CO + H2O	-103.8	A *	CONSIDER FORWARD FOR CHO BREAKDOWN
114R. CO + H2O = CHO + HO	103.8	C	REVERSE HIGHLY ENDOTHERMIC
115F. CHO + HO = CO2 + H2	-110.0	C	FOUR-CENTER REACTION
115R. CO2 + H2 = CHO + HO	110.0	C	CHO + HO = CO + H2O FASTER THAN FORWARD
			REVERSE HIGHLY ENDOTHERMIC
116F. CHO + HO2 = CH2O + O2	-39.1	B *	CONSIDER BOTH DIRECTIONS
116R. CH2O + O2 = CHO + HO2	39.1	B *	
117F. CHO + HO2 = CO2 + H2O	-165.1	C	FOUR-CENTER REACTION
117R. CO2 + H2O = CHO + HO2	165.1	C	CHO + HO2 = CH2O + O2 FASTER THAN FWD
			REVERSE HIGHLY ENDOTHERMIC
118F. CHO + H2 = CH2 + HO	92.8	C	FOUR-CENTER REACTION
118R. CH2 + HO = CHO + H2	-92.8	C	FORWARD ENDOTHERMIC
			CH3 + O AND CH2O + O MORE LIKELY
			PRODUCTS FROM REVERSE
119F. CHO + H2 = CH2O + H	19.0	B *	CONSIDER BOTH DIRECTIONS
119R. CH2O + H = CHO + H2	-19.0	A *	REVERSE MORE LIKELY TO BE IMPORTANT
			CH2O BREAKDOWN
120F. CHO + H2 = CH3 + O	86.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
120R. CH3 + O = CHO + H2	-86.5	C	

REACTION	HR	NOTES	COMMENTS
121F. CHO + H2 + M = CH3O + M	-6.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
121R. CH3O + M = CHO + H2 + M	6.5	C	
122F. CHO + H2O = CH2 + HO2	147.8	C	FOUR-CENTER REACTION
122R. CH2 + HO2 = CHO + H2O	-147.8	C	FORWARD HIGHLY ENDOTHERMIC
			CH2 + HO2 = CH3 + O2 FASTER THAN REVERSE
123F. CHO + H2O = CH2O + HO	33.8	C	CHO + M = CO + H + M FASTER THAN FORWARD
123R. CH2O + HO = CHO + H2O	-33.8	A *	CONSIDER REVERSE FOR CH2O BREAKDOWN
124F. CHO + H2O = CH3 + O2	85.7	C	NOT LIKELY TO BE ELEMENTARY REACTION
124R. CH3 + O2 = CHO + H2O	-85.7	C	
125F. CHO + H2O = CH3O + O	114.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
125R. CH3O + O = CHO + H2O	-114.6	C	
126F. CHO + N = CN + HO	-9.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
126R. CN + HO = CHO + N	9.5	C	
127F. CHO + N = CO + HN	-59.4	B *	CONSIDER FORWARD
127R. CO + HN = CHO + N	59.4	C	REVERSE ENDOTHERMIC
128F. CHO + NO = CN + HO2	78.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
128R. CN + HO2 = CHO + NO	-78.5	C	
129F. CHO + NO = CO + HNO	-33.2	B *	CONSIDER BOTH DIRECTIONS
129R. CO + HNO = CHO + NO	33.2	B *	PROBABLY NOT MAJOR IMPORTANCE
130F. CHO + NO = CO2 + HN	-32.7	C	FOUR-CENTER REACTION
130R. CO2 + HN = CHO + NO	32.7	C	CHO + NO = CO + HNO FASTER THAN FORWARD
			REVERSE MINOR

REACTION	HR	NOTES	COMMENTS
131F. CHO + NO2 = CO2 + HNO	-85.9	C	FOUR-CENTER
131R. CO2 + HNO = CHO + NO2	85.9	C	STERIC HINDRANCE
132F. CHO + N2 = CN + HNO	119.4	C	NOT LIKELY TO BE ELEMENTARY REACTION
132R. CN + HNO = CHO + N2	-119.4	C	
133F. CHO + O = CO + HO	-86.8	A *	CONSIDER FORWARD FOR CHO BREAKDOWN
133R. CO + HO = CHO + O	86.8	C	REVERSE ENDOTHERMIC
134F. CHO + O = CO2 + H	-107.9	B *	CONSIDER FORWARD
134R. CO2 + H = CHO + O	107.9	C	REVERSE HIGHLY ENDOTHERMIC
135F. CHO + O2 = CO + HO2	-30.8	B *	CONSIDER BOTH DIRECTIONS
135R. CO + HO2 = CHO + O2	30.8	B *	FORWARD FOR CHO BREAKDOWN REVERSE PROBABLY LESS IMPORTANT
136F. CHO + O2 = CO2 + HO	-92.2	C	FOUR-CENTER REACTION
136R. CO2 + HO = CHO + O2	92.2	C	CHO + O2 = CO + HO2 FASTER THAN FORWARD REVERSE ENDOTHERMIC
137F. CH2 + CH2O = CH4 + CO	-111.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
137R. CH4 + CO = CH2 + CH2O	111.6	C	
138F. CH2 + CH3O = CH2O + CH3	-87.0	C	LARGE MOLECULES, LOW CONCENTRATIONS
138R. CH2O + CH3 = CH2 + CH3O	87.0	C	REVERSE ENDOTHERMIC LIKELY TO BE UNIMPORTANT
139F. CH2 + CH4 = CH3 + CH3	-4.4	B *	CONSIDER BOTH DIRECTIONS FUEL RICH
139R. CH3 + CH3 = CH2 + CH4	4.4	B *	MAY BE IMPORTANT EARLY STAGES
140F. CH2 + CO2 = CH2O + CO	-52.7	C	FORWARD RX UNIMPORTANT FOR CH2 OR CO2
140R. CH2O + CO = CH2 + CO2	52.7	C	REVERSE ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
141F. CH2 + H + M = CH3 + M	-112.5	C	THIRD ORDER, LOW CONCENTRATIONS FORWARD
141R. CH3 + M = CH2 + H + M	112.5	C	REVERSE HIGHLY ENDOTHERMIC
142F. CH2 + HN = CH3 + N	-33.6	C	LOW CONCENTRATIONS BOTH DIRECTIONS
142R. CH3 + N = CH2 + HN	33.6	C	
143F. CH2 + HNO = CH2O + HN	-52.2	C	CH2 + HNO = CH3 + NO MORE LIKELY FORWARD
143R. CH2O + HN = CH2 + HNO	52.2	C	REVERSE ENDOTHERMIC
144F. CH2 + HNO = CH3 + NO	-59.8	C	FORWARD RX UNIMPORTANT FOR CH2 OR HNO
144R. CH3 + NO = CH2 + HNO	59.8	C	REVERSE ENDOTHERMIC
145F. CH2 + HNO = CH3O + N	1.2	C	NOT LIKELY TO BE ELEMENTARY REACTION
145R. CH3O + N = CH2 + HNO	-1.2	C	
146F. CH2 + HO = CH2O + H	-73.8	B *	CONSIDER FORWARD
146R. CH2O + H = CH2 + HO	73.8	C	REVERSE ENDOTHERMIC
147F. CH2 + HO = CH3 + O	-6.2	B *	CONSIDER BOTH DIRECTIONS
147R. CH3 + O = CH2 + HO	6.2	B *	REVERSE FOR CH3 BREAKDOWN
148F. CH2 + HO + M = CH3O + M	-99.3	C	CH2O + H OR CH3 + O MORE LIKELY PRODUCTS
148R. CH3O + M = CH2 + HO + M	99.3	C	REVERSE ENDOTHERMIC
149F. CH2 + HO2 = CH2O + HO	-114.0	C	CH2 + HO2 = CH3 + O2 MORE LIKELY FORWARD
149R. CH2O + HO = CH2 + HO2	114.0	C	REVERSE HIGHLY ENDOTHERMIC
150F. CH2 + HO2 = CH3 + O2	-62.2	B *	CONSIDER FORWARD
150R. CH3 + O2 = CH2 + HO2	62.2	C	REVERSE ENDOTHERMIC

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          REACTION                 HR   NOTES               COMMENTS

151F. CH2 + HO2 = CH3O + O      -33.2   C     NOT LIKELY TO BE ELEMENTARY REACTION
151R. CH3O + O = CH2 + HO2       33.2   C

152F. CH2 + H2 = CH3 + H         -4.1   B *   CONSIDER BOTH DIRECTIONS
152R. CH3 + H = CH2 + H2          4.1   A *   REVERSE FOR CH3 BREAKDOWN FUEL RICH

153F. CH2 + H2 + M = CH4 + M   -112.2   C     NOT LIKELY TO BE ELEMENTARY REACTION
153R. CH4 + M = CH2 + H2 + M    112.2   C

154F. CH2 + H2O = CH2O + H2     -58.9   C     NOT LIKELY TO BE ELEMENTARY REACTION
154R. CH2O + H2 = CH2 + H2O      58.9   C     MIGHT BE FOUR-CENTER STERICALLY HINDERED

155F. CH2 + H2O = CH3 + HO       10.8   B *   CONSIDER BOTH DIRECTIONS
155R. CH3 + HO = CH2 + H2O      -10.8   A *   REVERSE FOR CH3 BREAKDOWN

156F. CH2 + H2O = CH3O + H       24.0   C     NOT LIKELY TO BE ELEMENTARY REACTION
156R. CH3O + H = CH2 + H2O      -24.0   C

157F. CH2 + H2O = CH4 + O         9.0   C     NOT LIKELY TO BE ELEMENTARY REACTION
157R. CH4 + O = CH2 + H2O        -9.0   C

158F. CH2 + N = CN + H2        -102.3   C     NOT LIKELY TO BE ELEMENTARY REACTION
158R. CN + H2 = CH2 + N         102.3   C

159F. CH2 + NO = CH2O + N       -26.0   B *   CONSIDER FORWARD FUEL RICH
159R. CH2O + N = CH2 + NO        26.0   C     REVERSE NOT LIKELY TO BE IMPORTANT

160F. CH2 + NO = CN + H2O       -69.3   C     NOT LIKELY TO BE ELEMENTARY REACTION
160R. CN + H2O = CH2 + NO        69.3   C
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REACTION	HR	NOTES	COMMENTS
161F. CH2 + NO2 = CH2O + NO	-105.4	C	LOW CONCENTRATIONS FORWARD
161R. CH2O + NO = CH2 + NO2	105.4	C	REVERSE HIGHLY ENDOTHERMIC
162F. CH2 + N2O = CH2O + N2	-140.2	C	LOW CONCENTRATIONS FORWARD
162R. CH2O + N2 = CH2 + N2O	140.2	C	REVERSE HIGHLY ENDOTHERMIC
163F. CH2 + O + M = CH2O + M	-180.1	C	THIRD ORDER FORWARD
163R. CH2O + M = CH2 + O + M	180.1	C	REVERSE HIGHLY ENDOTHERMIC
164F. CH2 + O = CO + H2	-179.5	C	NOT LIKELY TO BE ELEMENTARY REACTION
164R. CO + H2 = CH2 + O	179.5	C	
165F. CH2 + O2 = CH2O + O	-58.1	B *	CONSIDER FORWARD
165R. CH2O + O = CH2 + O2	58.1	C	REVERSE ENDOTHERMIC
166F. CH2 + O2 = CO + H2O	-178.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
166R. CO + H2O = CH2 + O2	178.6	C	
167F. CH2 + O2 = CO2 + H2	-184.9	C	NOT LIKELY TO BE ELEMENTARY REACTION
167R. CO2 + H2 = CH2 + O2	184.9	C	
168F. CH2O + M = CO + H2 + M	0.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
168R. CO + H2 + M = CH2O + M	-0.6	C	
169F. CH2O + CH2O = CH4 + CO2	-59.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
169R. CH4 + CO2 = CH2O + CH2O	59.0	C	
170F. CH2O + CH4 = CH3 + CH3O	82.7	C	FORWARD ENDOTHERMIC
170R. CH3 + CH3O = CH2O + CH4	-82.7	C	LARGE MOLECULES LOW CONCENTRATIONS REV

	REACTION	HR	NOTES	COMMENTS
171F.	CH2O + H = CH3 + O	67.6	C	FORWARD ENDOTHERMIC
171R.	CH3 + O = CH2O + H	-67.6	A *	CONSIDER REVERSE FOR CH3 BREAKDOWN
172F.	CH2O + H + M = CH3O + M	-25.5	B *	CONSIDER BOTH DIRECTIONS
172R.	CH3O + M = CH?O + H + M	25.5	B *	REVERSE MAY BE IMPORTANT CH3O BREAKDOWN
173F.	CH2O + HN = CH3 + NO	-7.6	C	FOUR-CENTER, STERIC HINDRANCE
173R.	CH3 + NO = CH2O + HN	7.6	C	
174F.	CH2O + HN = CH3O + N	53.4	C	FORWARD ENDOTHERMIC
174R.	CH3O + N = CH2O + HN	-53.4	B *	CONSIDER REVERSE FOR CH3O BREAKDOWN PROBABLY MINOR
175F.	CH2O + HNO = CH3 + NO2	45.6	C	FOUR-CENTER, STERIC HINDRANCE
175R.	CH3 + NO2 = CH2O + HNO	-45.6	C	
176F.	CH2O + HNO = CH3O + NO	27.2	C	LOW CONCENTRATIONS BOTH DIRECTIONS
176R.	CH3O + NO = CH2O + HNO	-27.2	C	
177F.	CH2O + HO = CH3 + O2	51.8	C	FORWARD ENDOTHERMIC
177R.	CH3 + O2 = CH2O + HO	-51.8	B *	CONSIDER REVERSE FOR CH3 BREAKDOWN FOUR-CENTER REACTION
178F.	CH2O + HO = CH3O + O	80.8	C	FORWARD ENDOTHERMIC
178R.	CH3O + O = CH2O + HO	-80.8	B *	CONSIDER REVERSE FOR CH3O BREAKDOWN
179F.	CH2O + HO2 = CH3O + O2	24.9	C	LOW CONCENTRATIONS FORWARD
179R.	CH3O + O2 = CH2O + HO2	-24.9	B *	CONSIDER REVERSE FOR CH3O BREAKDOWN
180F.	CH2O + H2 = CH3 + HO	69.7	C	FOUR-CENTER REACTION
180R.	CH3 + HO = CH2O + H2	-69.7	C	FORWARD ENDOTHERMIC CH3 + HO = CH4 + O AND CH3 + HO = CH2 + H2O MORE LIKELY REVERSE

REACTION	HR	NOTES	COMMENTS
181F. CH2O + H2 = CH3O + H	83.0	C	FORWARD ENDOTHERMIC
181R. CH3O + H = CH2O + H2	-83.0	B *	CONSIDER REVERSE FOR CH3O BREAKDOWN
182F. CH2O + H2 = CH4 + O	67.9	C	NOT LIKELY TO BE ELEMENTARY REACTION
182R. CH4 + O = CH2O + H2	-67.9	C	
183F. CH2O + H2O = CH3 + HO2	124.8	C	FOUR-CENTER REACTION
183R. CH3 + HO2 = CH2O + H2O	-124.8	C	STERIC HINDRANCE
184F. CH2O + H2O = CH3O + HO	97.8	C	FORWARD ENDOTHERMIC
184R. CH3O + HO = CH2O + H2O	-97.8	B *	CONSIDER REVERSE FOR CH3O BREAKDOWN
185F. CH2O + H2O = CH4 + O2	67.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
185R. CH4 + O2 = CH2O + H2O	-67.0	C	
186F. CH2O + N = CN + H2O	-43.3	C	NOT LIKELY TO BE ELEMENTARY REACTION
186R. CN + H2O = CH2O + N	43.3	C	
187F. CH2O + O = CO + H2O	-120.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
187R. CO + H2O = CH2O + O	120.6	C	
188F. CH2O + O = CO2 + H2	-126.8	C	NOT LIKELY TO BE ELEMENTARY REACTION
188R. CO2 + H2 = CH2O + O	126.8	C	
189F. CH2O + O2 = CO2 + H2O	-126.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
189R. CO2 + H2O = CH2O + O2	126.0	C	
190F. CH3 + CO2 = CH3O + CO	34.4	C	LARGE MOLECULES
190R. CH3O + CO = CH3 + CO2	-34.4	C	LIKELY TO BE UNIMPORTANT

REACTION	HR	NOTES	COMMENTS
191F. CH3 + H + M = CH4 + M	-108.2	B *	MAY BE IMPORTANT EARLY STAGES
191R. CH4 + M = CH3 + H + M	108.2	B *	
192F. CH3 + HN = CH4 + N	-29.2	C	LOW CONCENTRATIONS
192R. CH4 + N = CH3 + HN	29.2	C	
193F. CH3 + HNO = CH3O + HN	34.8	C	LOW CONCENTRATIONS
193R. CH3O + HN = CH3 + HNO	-34.8	C	
194F. CH3 + HNO = CH4 + NO	-55.4	C	LOW CONCENTRATIONS FORWARD
194R. CH4 + NO = CH3 + HNO	55.4	C	REVERSE ENDOTHERMIC
195F. CH3 + HO = CH3O + H	13.2	B *	CONSIDER BOTH DIRECTIONS FOR ROLE CH3O
195R. CH3O + H = CH3 + HO	-13.2	B *	
196F. CH3 + HO = CH4 + O	-1.8	A *	CONSIDER BOTH DIRECTIONS
196R. CH4 + O = CH3 + HO	1.8	A *	ROLE IN INITIAL CH4 BREAKDOWN
197F. CH3 + HO2 = CH3O + HO	-27.0	C	CH3 + HO2 = CH4 + O2 MORE LIKELY FORWARD
197R. CH3O + HO = CH3 + HO2	27.0	C	CH3O + HO = CH2O + H2O MORE LIKELY REV
198F. CH3 + HO2 = CH4 + O2	-57.8	B *	CONSIDER FORWARD
198R. CH4 + O2 = CH3 + HO2	57.8	C	REVERSE ENDOTHERMIC
199F. CH3 + H2 = CH4 + H	0.3	A *	CONSIDER BOTH DIRECTIONS
199R. CH4 + H = CH3 + H2	-0.3	A *	ROLE IN INITIAL CH4 BREAKDOWN
200F. CH3 + H2O = CH3O + H2	28.1	C	NOT LIKELY TO BE ELEMENTARY REACTION
200R. CH3O + H2 = CH3 + H2O	-28.1	C	

REACTION	HR	NOTES	COMMENTS
201F. CH3 + H2O = CH4 + HO	15.2	A *	CONSIDER BOTH DIRECTIONS
201R. CH4 + HO = CH3 + H2O	-15.2	A *	ROLE IN INITIAL CH4 BREAKDOWN
202F. CH3 + NO = CH3O + N	61.0	C	FORWARD ENDOTHERMIC
202R. CH3O + N = CH3 + NO	-61.0	C	CH3O + N = CH2O + HN MORE LIKELY REVERSE
203F. CH3 + NO2 = CH3O + NO	-18.3	C	LOW CONCENTRATIONS BOTH DIRECTIONS
203R. CH3O + NO = CH3 + NO2	18.3	C	
204F. CH3 + N2O = CH3O + N2	-53.2	C	LARGE MOLECULES STERIC HINDRANCE FORWARD
204R. CH3O + N2 = CH3 + N2O	53.2	C	REVERSE ENDOTHERMIC
205F. CH3 + O + M = CH3O + M	-93.1	C	THIRD ORDER FORWARD
205R. CH3O + M = CH3 + O + M	93.1	C	STABILIZATION UNLIKELY REVERSE ENDOTHERMIC
206F. CH3 + O2 = CH3O + O	29.0	B *	CONSIDER BOTH DIRECTIONS
206R. CH3O + O = CH3 + O2	-29.0	B *	FORWARD FOR CH3 BREAKDOWN
207F. CH3O + H = CH4 + O	-15.1	C	CH3O + H = CH2O + H2 MORE LIKELY FORWARD
207R. CH4 + O = CH3O + H	15.1	C	CH4 + O = CH3 + HO MORE LIKELY REVERSE
208F. CH3O + HN = CH4 + NO	-90.3	C	LOW CONCENTRATIONS FORWARD
208R. CH4 + NO = CH3O + HN	90.3	C	REVERSE ENDOTHERMIC
209F. CH3O + HNO = CH4 + NO2	-37.1	C	LOW CONCENTRATIONS BOTH DIRECTIONS
209R. CH4 + NO2 = CH3O + HNO	37.1	C	FOUR-CENTER, STERIC HINDRANCE
210F. CH3O + HO = CH4 + O2	-30.8	C	FOUR-CENTER, STERIC HINDRANCE
210R. CH4 + O2 = CH3O + HO	30.8	C	

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          REACTION                  HR    NOTES              COMMENTS

211F. CH3O + H2 = CH4 + HO       -12.9    C     FOUR-CENTER, STERIC HINDRANCE
211R. CH4 + HO = CH3O + H2        12.9    C

212F. CH3O + H2O = CH4 + HO2      42.1    C     FOUR-CENTER, STERIC HINDRANCE
212R. CH4 + HO2 = CH3O + H2O     -42.1    C

213F. CN + HO = CO + HN          -49.9    C     FOUR-CENTER REACTION
213R. CO + HN = CN + HO           49.9    C     CN + HO = CHN + O MORE LIKELY FORWARD
                                                REVERSE ENDOTHERMIC

214F. CN + HO2 = CO + HNO       -111.7    C     FOUR-CENTER FOR NOH STRUCTURE
214R. CO + HNO = CN + HO2        111.7    C     REVERSE HIGHLY ENDOTHERMIC

215F. CN + HO2 = CO2 + HN       -111.2    C     NOT LIKELY TO BE ELEMENTARY REACTION
215R. CO2 + HN = CN + HO2        111.2    C

216F. CN + NO = CO + N2         -152.6    B *   CONSIDER FORWARD FOR NO DESTRUCTION
216R. CO + N2 = CN + NO          152.6    C     REVERSE HIGHLY ENDOTHERMIC
                                                FOUR-CENTER REACTION

217F. CN + NO2 = CO + N2O       -117.7    C     FOUR-CENTER, STERIC HINDRANCE
217R. CO + N2O = CN + NO2        117.7    C     REVERSE HIGHLY ENDOTHERMIC

218F. CN + NO2 = CO2 + N2       -205.3    C     NOT LIKELY TO BE ELEMENTARY REACTION
218R. CO2 + N2 = CN + NO2        205.3    C

219F. CN + O = CO + N            -77.2    B *   CONSIDER FORWARD
219R. CO + N = CN + O             77.2    C     REVERSE ENDOTHERMIC

220F. CN + O2 = CO + NO         -109.3    B *   FOUR-CENTER REACTION, PROBABLY SLOW
220R. CO + NO = CN + O2          109.3    C     REVERSE HIGHLY ENDOTHERMIC
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REACTION	HR	NOTES	COMMENTS
221F. CN + O2 = CO2 + N	-82.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
221R. CO2 + N = CN + O2	82.6	C	
222F. CO + HNO = CO2 + HN	0.4	C	HNO, HN MINOR RX PARTNERS FOR CO, CO2
222R. CO2 + HN = CO + HNO	-0.4	C	
223F. CO + HO = CO2 + H	-21.1	A *	FORWARD MAIN PATH FROM CO TO CO2
223R. CO2 + H = CO + HO	21.1	B *	CONSIDER BOTH DIRECTIONS
224F. CO + HO2 = CO2 + HO	-61.3	C	CO + HO = CO2 + H MORE IMPORTANT FORWARD
224R. CO2 + HO = CO + HO2	61.3	C	MAY HAVE MINOR ROLE FORWARD REVERSE ENDOTHERMIC
225F. CO + H2O = CO2 + H2	-6.3	C	NOT LIKELY TO BE ELEMENTARY REACTION
225R. CO2 + H2 = CO + H2O	6.3	C	
226F. CO + NO = CO2 + N	26.7	C	SPIN HINDERED
226R. CO2 + N = CO + NO	-26.7	C	EXPERIMENT INDICATES REACTION SLOW
227F. CO + NO2 = CO2 + NO	-52.7	C	LOW CONCENTRATIONS FORWARD
227R. CO2 + NO = CO + NO2	52.7	C	REVERSE ENDOTHERMIC
228F. CO + N2O = CO2 + N2	-87.6	C	CO, N2O MINOR REACTION PARTNERS
228R. CO2 + N2 = CO + N2O	87.6	C	REVERSE ENDOTHERMIC
229F. CO + O + M = CO2 + M	-127.4	B *	FORWARD TERMINATION REACTION
229R. CO2 + M = CO + O + M	127.4	C	REVERSE HIGHLY ENDOTHERMIC
230F. CO + O2 = CO2 + O	-5.4	B *	CONSIDER BOTH DIRECTIONS
230R. CO2 + O = CO + O2	5.4	B *	PROBABLY SLOWER THAN CO + HO = CO2 + H

REACTION	HR	NOTES	COMMENTS
231F. H + H + M = H2 + M	-108.4	A *	FORWARD TERMINATION REACTION
231R. H2 + M = H + H + M	108.4	C	REVERSE HIGHLY ENDOTHERMIC
232F. H + HN = H2 + N	-29.5	B *	CONSIDER BOTH DIRECTIONS
232R. H2 + N = H + HN	29.5	B *	
233F. H + HNO = HN + HO	21.6	B *	CONSIDER BOTH DIRECTIONS
233R. HN + HO = H + HNO	-21.6	B *	PROBABLY MINOR
234F. H + HNO = H2 + NO	-55.7	B *	CONSIDER FORWARD, PROBABLY MINOR
234R. H2 + NO = H + HNO	55.7	C	REVERSE ENDOTHERMIC
235F. H + HNO = H2O + N	-22.8	C	POSSIBLE FOR NOH STRUCTURE
235R. H2O + N = H + HNO	22.8	C	PROBABLY MINOR
236F. H + HO = H2O + O	-2.2	A *	CONSIDER BOTH DIRECTIONS
236R. H2O + O = H + HO	2.2	A *	
237F. H + HO + M = H2O + M	-123.3	A *	FORWARD TERMINATION REACTION
237R. H2O + M = H + HO + M	123.3	C	REVERSE HIGHLY ENDOTHERMIC
238F. H + HO2 = HO + HO	-40.2	B *	CONSIDER FORWARD FOR HO2 REMOVAL
238R. HO + HO = H + HO2	40.2	C	HO + HO = H2O + O FASTER THAN REVERSE
239F. H + HO2 = H2 + O2	-58.1	B *	CONSIDER FORWARD FOR HO2 REMOVAL
239R. H2 + O2 = H + HO2	58.1	C	REVERSE ENDOTHERMIC
240F. H + HO2 = H2O + O	-57.2	C	FORWARD PRODUCTS MORE LIKELY TO BE
240R. H2O + O = H + HO2	57.2	C	HO + HO OR H2 + O2

REACTION	HR	NOTES	COMMENTS
241F. H + H2O = HO + H2	14.9	A *	CONSIDER BOTH DIRECTIONS
241R. HO + H2 = H + H2O	-14.9	A *	
242F. H + N + M = HN + M	-78.9	C	THIRD ORDER, LOW CONCENTRATIONS FORWARD
242R. HN + M = H + N + M	78.9	C	REVERSE ENDOTHERMIC
243F. H + NO = HN + O	75.9	C	FORWARD ENDOTHERMIC
243R. HN + O = H + NO	-75.9	B *	CONSIDER REVERSE
244F. H + NO + M = HNO + M	-52.7	C	THIRD ORDER FORWARD
244R. HNO + M = H + NO + M	52.7	C	REVERSE ENDOTHERMIC
245F. H + NO = HO + N	47.8	B *	CONSIDER BOTH DIRECTIONS
245R. HO + N = H + NO	-47.8	A *	REVERSE PART OF MODIFIED ZELDOVICH
246F. H + NO2 = HN + O2	27.9	C	STERIC HINDRANCE
246R. HN + O2 = H + NO2	-27.9	C	OTHER PRODUCTS MORE LIKELY
247F. H + NO2 = HNO + O	22.0	C	POSSIBLE FOR NOH STRUCTURE
247R. HNO + O = H + NO2	-22.0	C	OTHER PRODUCTS MORE LIKELY
248F. H + NO2 = HO + NO	-31.6	B *	CONSIDER BOTH DIRECTIONS
248R. HO + NO = H + NO2	31.6	B *	PROBABLY UNIMPORTANT
249F. H + NO2 = HO2 + N	56.4	C	NOT LIKELY TO BE ELEMENTARY REACTION
249R. HO2 + N = H + NO2	-56.4	C	
250F. H + N2 = HN + N	150.5	C	FORWARD HIGHLY ENDOTHERMIC
250R. HN + N = H + N2	-150.5	C	LOW CONCENTRATIONS REVERSE

REACTION	HR	NOTES	COMMENTS
251F. H + N2O = HN + NO	36.2	C	H + N2O = HO + N2 FASTER FORWARD
251R. HN + NO = H + N2O	-36.2	C	LOW CONCENTRATIONS REVERSE
252F. H + N2O = HNO + N	62.5	C	FORWARD ENDOTHERMIC
252R. HNO + N = H + N2O	-62.5	C	LOW CONCENTRATIONS REVERSE
253F. H + N2O = HO + N2	-66.4	B *	CONSIDER FORWARD
253R. HO + N2 = H + N2O	66.4	C	REVERSE ENDOTHERMIC
254F. H + O + M = HO + M	-106.3	A *	FORWARD REMOVES ACTIVE CENTERS
254R. HO + M = H + O + M	106.3	C	REVERSE HIGHLY ENDOTHERMIC
255F. H + O2 = HO + O	15.7	A *	CONSIDER BOTH DIRECTIONS
255R. HO + O = H + O2	-15.7	A *	
256F. H + O2 + M = HO2 + M	-50.4	B *	CONSIDER FORWARD
256R. HO2 + M = H + O2 + M	50.4	C	REVERSE ENDOTHERMIC
257F. HN + HN = H2 + N2	-180.0	C	FOUR-CENTER REACTION
257R. H2 + N2 = HN + HN	180.0	C	LOW CONCENTRATIONS FORWARD
			REVERSE HIGHLY ENDOTHERMIC
258F. HN + HNO = H2 + N2O	-92.0	C	FOUR-CENTER, STERIC HINDRANCE
258R. H2 + N2O = HN + HNO	92.0	C	LOW CONCENTRATIONS FORWARD
			REVERSE ENDOTHERMIC
259F. HN + HNO = H2O + N2	-173.3	C	FOUR-CENTER, STERIC HINDRANCE
259R. H2O + N2 = HN + HNO	173.3	C	
260F. HN + HO = H2 + NO	-77.3	C	FOUR-CENTER REACTION
260R. H2 + NO = HN + HO	77.3	C	HN + HO = H2O + N MORE LIKELY FORWARD
			REVERSE ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
261F. HN + HO = H2O + N	-44.4	B *	CONSIDER FORWARD
261R. H2O + N = HN + HO	44.4	C	REVERSE ENDOTHERMIC
262F. HN + HO2 = HNO + HO	-61.8	C	LOW CONCENTRATIONS FORWARD
262R. HNO + HO = HN + HO2	61.8	C	REVERSE ENDOTHERMIC
263F. HN + HO2 = H2 + NO2	-86.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
263R. H2 + NO2 = HN + HO2	86.0	C	
264F. HN + HO2 = H2O + NO	-132.4	C	FOUR-CENTER REACTION, STERIC HINDRANCE
264R. H2O + NO = HN + HO2	132.4	C	
265F. HN + H2O = HNO + H2	-6.7	C	FOUR-CENTER REACTION STERIC HINDRANCE
265R. HNO + H2 = HN + H2O	6.7	C	NOH STRUCTURE
266F. HN +.NO = HNO + N	26.2	C	LOW CONCENTRATIONS BOTH DIRECTIONS
266R. HNO + N = HN +.NO	-26.2	C	
267F. HN + NO = HO + N2	-102.7	C	FOUR-CENTER REACTION
267R. HO + N2 = HN + NO	102.7	C	LOW CONCENTRATIONS FORWARD
			REVERSE HIGHLY ENDOTHERMIC
268F. HN + NO2 = HNO + NO	-53.2	C	LOW CONCENTRATIONS BOTH DIRECTIONS
268R. HNO + NO = HN + NO2	53.2	C	
269F. HN + NO2 = HO + N2O	-67.8	C	FOUR-CENTER REACTION, STERIC HINDRANCE
269R. HO + N2O = HN + NO2	67.8	C	LOW CONCENTRATIONS FORWARD
			REVERSE ENDOTHERMIC
270F. HN + NO2 = HO2 + N2	-94.0	C	NOT LIKELY TO BE ELEMENTARY REACTION
270R. HO2 + N2 = HN + NO2	94.0	C	

REACTION	HR	NOTES	COMMENTS
271F. HN + N2O = HNO + N2	-88.0	C	LOW CONCENTRATIONS FORWARD
271R. HNO + N2 = HN + N2O	88.0	C	REVERSE ENDOTHERMIC
272F. HN + O + M = HNO + M	-127.9	C	THIRD ORDER FORWARD
272R. HNO + M = HN + O + M	127.9	C	REVERSE HIGHLY ENDOTHERMIC
273F. HN + O = HO + N	-27.4	C	HN + O = H + NO MORE LIKELY FORWARD
273R. HO + N = HN + O	27.4	C	HO + N = H + NO MORE LIKELY REVERSE
274F. HN + O2 = HNO + O	-5.8	B *	CONSIDER BOTH DIRECTIONS
274R. HNO + O = HN + O2	5.8	B *	PROBABLY MINOR
275F. HN + O2 = HO + NO	-59.4	C	FOUR-CENTER REACTION
275R. HO + NO = HN + O2	59.4	C	HN + O2 = HNO + O FASTER FORWARD REVERSE ENDOTHERMIC
276F. HN + O2 = HO2 + N	28.6	C	HN + O2 = HNO + O FASTER FORWARD
276R. HO2 + N = HN + O2	-28.6	C	LOW CONCENTRATIONS REVERSE
277F. HNO + M = HO + N + M	100.5	C	FORWARD HIGHLY ENDOTHERMIC
277R. HO + N + M = HNO + M	-100.5	C	THIRD ORDER REVERSE NOH STRUCTURE
278F. HNO + HNO = H2O + N2O	-85.3	C	FOUR-CENTER REACTION, STERIC HINDRANCE
278R. H2O + N2O = HNO + HNO	85.3	C	
279F. HNO + HO = H2 + NO2	-24.2	C	FOUR-CENTER REACTION
279R. H2 + NO2 = HNO + HO	24.2	C	HNO + HO = H2O + NO MORE LIKELY FORWARD LOW CONCENTRATIONS REVERSE
280F. HNO + HO = H2O + NO	-70.6	B *	CONSIDER FORWARD
280R. H2O + NO = HNO + HO	70.6	C	REVERSE ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
281F. HNO + HO2 = H2O + NO2	-79.2	C	FOUR-CENTER REACTION, STERIC HINDRANCE
281R. H2O + NO2 = HNO + HO2	79.2	C	
282F. HNO + N = HO + N2	-128.9	C	LOW CONCENTRATIONS FORWARD
282R. HO + N2 = HNO + N	128.9	C	REVERSE HIGHLY ENDOTHERMIC
283F. HNO + NO = HO + N2O	-14.7	C	FOUR-CENTER REACTION, STERIC HINDRANCE
283R. HO + N2O = HNO + NO	14.7	C	
284F. HNO + NO = HO2 + N2	-40.9	C	FOUR-CENTER REACTION, NOH STRUCTURE
284R. HO2 + N2 = HNO + NO	40.9	C	LOW CONCENTRATIONS FORWARD REVERSE ENDOTHERMIC
285F. HNO + NO2 = HO2 + N2O	-6.0	C	FOUR-CENTER REACTION, STERIC HINDRANCE
285R. HO2 + N2O = HNO + NO2	6.0	C	
286F. HNO + O = HO + NO	-53.6	B *	CONSIDER FORWARD
286R. HO + NO = HNO + O	53.6	C	REVERSE ENDOTHERMIC
287F. HNO + O = HO2 + N	34.4	C	HNO + O = HO + NO FASTER FORWARD
287R. HO2 + N = HNO + O	-34.4	C	LOW CONCENTRATIONS REVERSE
288F. HNO + O2 = HO + NO2	-6.3	C	FOUR-CENTER REACTION, STERIC HINDRANCE
288R. HO + NO2 = HNO + O2	6.3	C	
289F. HNO + O2 = HO2 + NO	2.4	C	FOUR-CENTER REACTION, STERIC HINDRANCE
289R. HO2 + NO = HNO + O2	-2.4	C	
290F. HO + HO = H2 + O2	-17.9	C	FOUR-CENTER REACTION
290R. H2 + O2 = HO + HO	17.9	C	HO + HO = H2O + O FASTER FORWARD REVERSE MAY HAVE ROLE IN H2/O2 IGNITION

REACTION	HR	NOTES	COMMENTS
291F. HO + HO = H2O + O	-17.0	A *	CONSIDER BOTH DIRECTIONS
291R. H2O + O = HO + HO	17.0	A *	
292F. HO + HO2 = H2O + O2	-73.0	A *	CONSIDER FORWARD FOR HO2 REMOVAL
292R. H2O + O2 = HO + HO2	73.0	C	REVERSE ENDOTHERMIC
293F. HO + H2O = HO2 + H2	55.1	C	FOUR-CENTER REACTION
29´R. HO2 + H2 = HO + H2O	-55.1	C	FORWARD ENDOTHERMIC
294F. HO + NO = HO2 + N	88.0	C	FORWARD ENDOTHERMIC
294R. HO2 + N = HO + NO	-88.0	C	LOW CONCENTRATIONS REVERSE
295F. HO + NO2 = HO2 + NO	8.6	B *	CONSIDER BOTH DIRECTIONS
295R. HO2 + NO = HO + NO2	-8.6	B *	REVERSE HAS BEEN CONSIDERED FOR EARLY NO2 FORMATION
296F. HO + N2O = HO2 + N2	-26.2	B *	CONSIDER BOTH DIRECTIONS
296R. HO2 + N2 = HO + N2O	26.2	B *	PROBABLY MINOR
297F. HO + O + M = HO2 + M	-66.1	B *	CONSIDER FORWARD
297R. HO2 + M = HO + O + M	66.1	C	REVERSE ENDOTHERMIC
298F. HO + O2 = HO2 + O	55.9	C	FORWARD ENDOTHERMIC
298R. HO2 + O = HO + O2	-55.9	A *	CONSIDER REVERSE FOR HO2 REMOVAL
299F. H2 + NO = H2O + N	32.9	C	NOT LIKELY TO BE ELEMENTARY REACTION
299R. H2O + N = H2 + NO	-32.9	C	
300F. H2 + NO2 = H2O + NO	-46.4	C	NOT LIKELY TO BE ELEMENTARY REACTION
300R. H2O + NO = H2 + NO2	46.4	C	

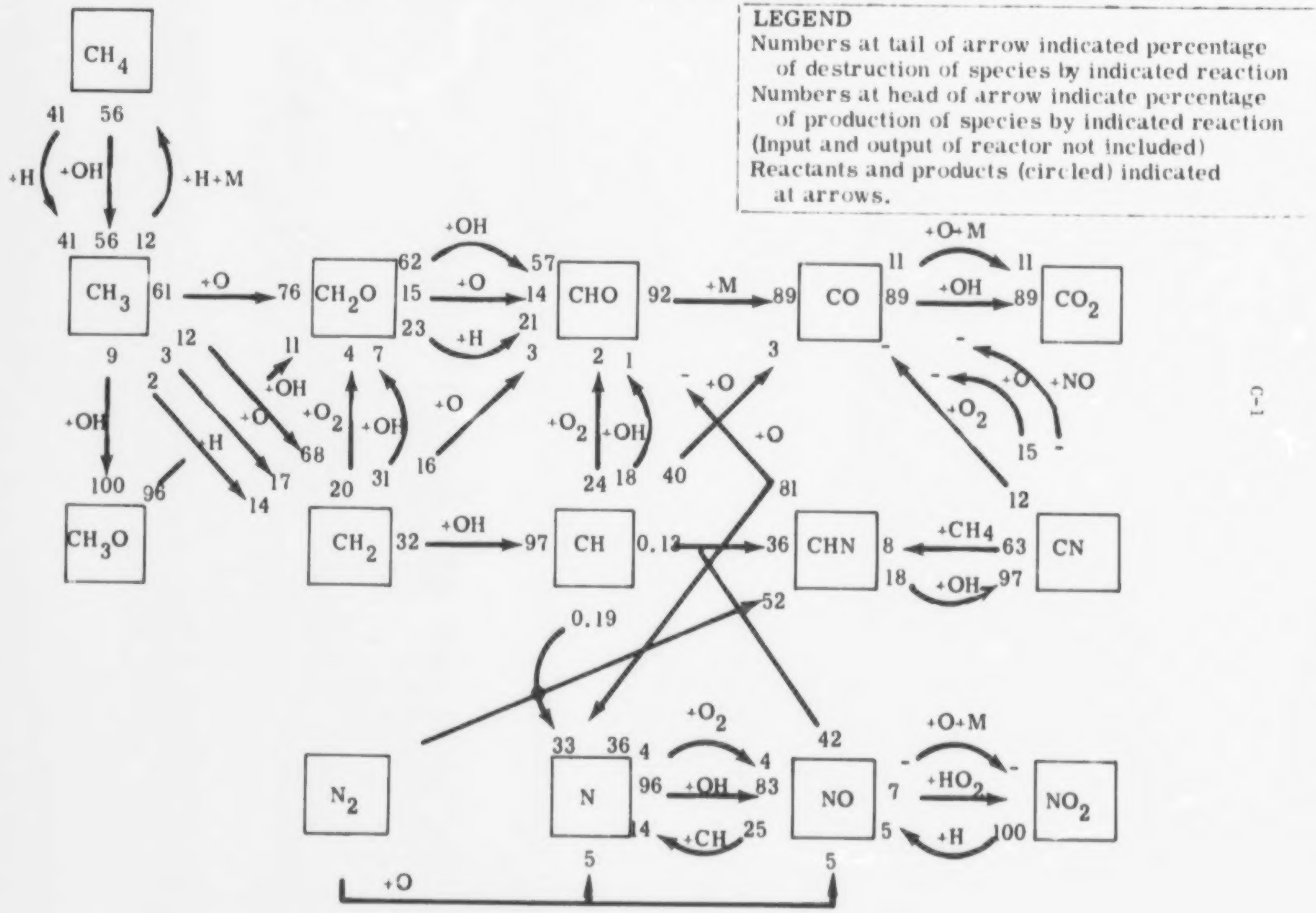
REACTION	HR	NOTES	COMMENTS
301F. H2 + N2O = H2O + N2	-81.3	C	NOT LIKELY TO BE ELEMENTARY REACTION
301R. H2O + N2 = H2 + N2O	81.3	C	
302F. H2 + O + M = H2O + M	-121.2	C	NOT LIKELY TO BE ELEMENTARY REACTION
302R. H2O + M = H2 + O + M	121.2	C	
303F. H2 + O2 = H2O + O	0.9	C	NOT LIKELY TO BE ELEMENTARY REACTION
303R. H2O + O = H2 + O2	-0.9	C	
304F. N + N + M = N2 + M	-229.4	C	THIRD ORDER, LOW CONCENTRATIONS FORWARD
304R. N2 + M = N + N + M	229.4	C	REVERSE HIGHLY ENDOTHERMIC
305F. N + NO = N2 + O	-75.3	B *	CONSIDER BOTH DIRECTIONS
305R. N2 + O = N + NO	75.3	A *	REVERSE PART OF ZELDOVICH MECHANISM
306F. N + NO + M = N2O + M	-115.2	C	THIRD ORDER, LOW CONCENTRATIONS FORWARD
306R. N2O + M = N + NO + M	115.2	C	REVERSE HIGHLY ENDOTHERMIC
307F. N + NO2 = NO + NO	-79.4	B *	CONSIDER FORWARD (LOW CONCENTRATIONS)
307R. NO + NO = N + NO2	79.4	C	REVERSE ENDOTHERMIC
308F. N + NO2 = N2 + O2	-122.6	C	NOT LIKELY TO BE ELEMENTARY REACTION
308R. N2 + O2 = N + NO2	122.6	C	
309F. N NO2 = N2O + O	-40.4	C	N + NO2 = NO + NO MORE LIKELY FORWARD
309R. N2O + O = N + NO2	40.4	C	REVERSE ENDOTHERMIC
310F. N + N2O = NO + N2	-114.2	C	LOW CONCENTRATIONS FORWARD
310R. NO + N2 = N + N2O	114.2	C	REVERSE HIGHLY ENDOTHERMIC

REACTION	HR	NOTES	COMMENTS
311F. N + O + M = NO + M	-154.1	C	THIRD ORDER, LOW CONCENTRATION FORWARD
311R. NO + M = N + O + M	154.1	C	REVERSE HIGHLY ENDOTHERMIC
312F. N + O2 = NO + O	-32.1	A *	CONSIDER BOTH DIRECTIONS
312R. NO + O = N + O2	32.1	B *	FORWARD PART OF ZELDOVICH MECHANISM
313F. N + O2 + M = NO2 + M	-106.8	C	NOT LIKELY TO BE ELEMENTARY REACTION
313R. NO2 + M = N + O2 + M	106.8	C	
314F. NO + NO = N2 + O2	-43.2	C	FOUR-CENTER REACTION, SPIN HINDERED
314R. N2 + O2 = NO + NO	43.2	C	NO + NO = N2O + O FASTER EXPERIMENTALLY
			POSSIBLY BY AT LEAST A FACTOR OF 10
315F. NO + NO = N2O + O	38.9	B *	CONSIDER BOTH DIRECTIONS
315R. N2O + O = NO + NO	-38.9	B *	
316F. NO + NO2 = N2O + O2	-8.4	C	NOT LIKELY TO BE ELEMENTARY REACTION
316R. N2O + O2 = NO + NO2	8.4	C	
317F. NO + N2O = NO2 + N2	-34.9	C	FORWARD SLOW EXPERIMENTALLY
317R. NO2 + N2 = NO + N2O	34.9	C	REVERSE EVEN SLOWER
318F. NO + O + M = NO2 + M	-74.7	B *	CONSIDER FORWARD
318R. NO2 + M = NO + O + M	74.7	C	REVERSE ENDOTHERMIC
319F. NO + O2 = NO2 + O	47.3	B *	CONSIDER BOTH DIRECTIONS
319R. NO2 + O = NO + O2	-47.3	B *	FORWARD ENDOTHERMIC
320F. N2 + O + M = N2O + M	-39.9	B *	CONSIDER BOTH DIRECTIONS FOR ROLE OF N2O
320R. N2O + M = N2 + O + M	39.9	B *	

REACTION	HR	NOTES	COMMENTS
321F. N2 + O2 = N2O + O	82.2	C	FORWARD ENDOTHERMIC
321R. N2O + O = N2 + O2	-82.2	B *	CONSIDER REVERSE
322F. O + O + M = O2 + M	-122.0	A *	FORWARD TERMINATION REACTION
322R. O2 + M = O + O + M	122.0	C	REVERSE HIGHLY ENDOTHERMIC

FIGURE C-1

MAJOR KINETIC PATHS FOR METHANE AIR COMBUSTION COUPLED TO NO_X FORMATION
STIRRED REACTOR, 80% STOICHIOMETRIC AIR, τ = 2 msec

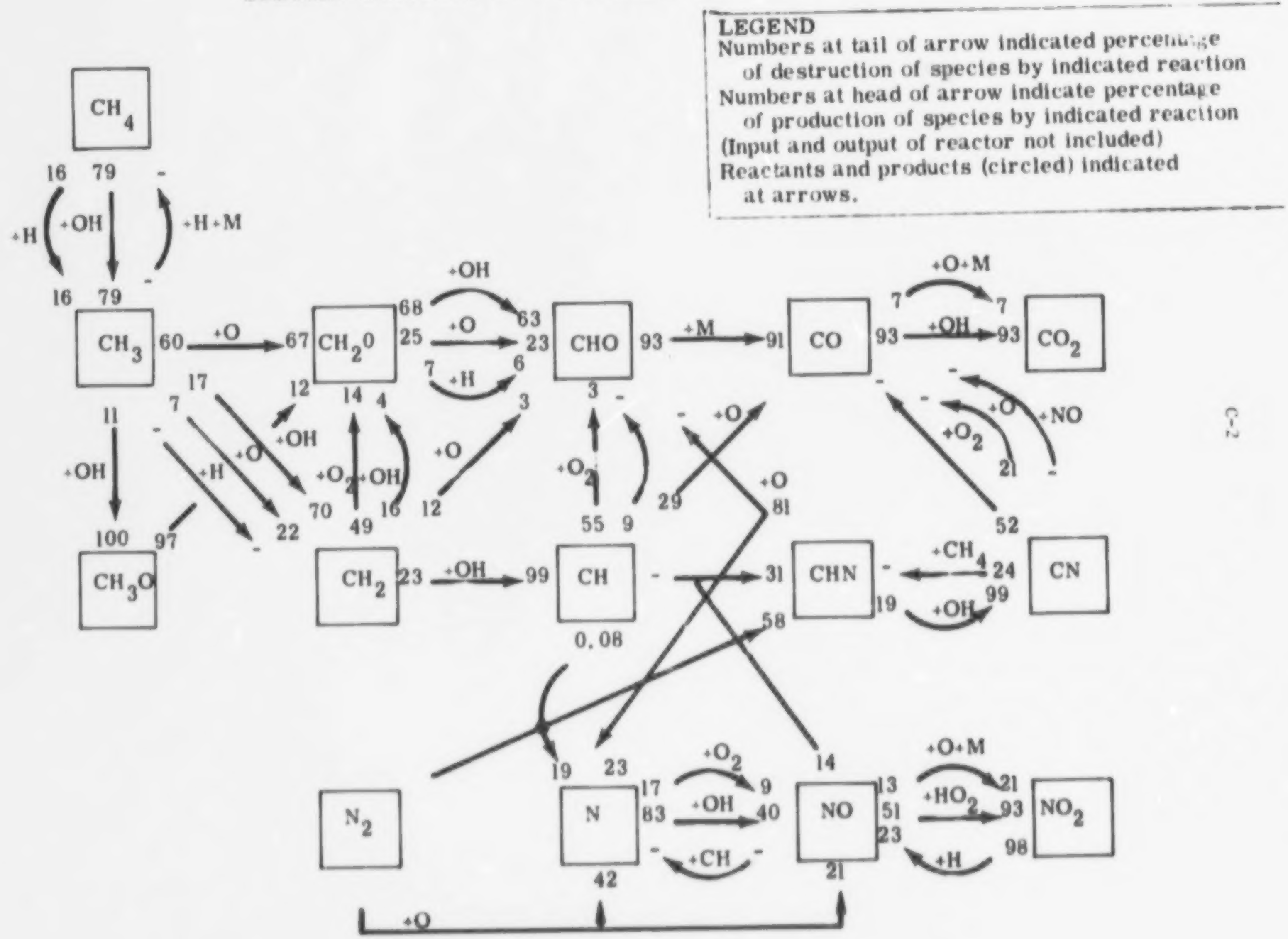


LEGEND
Numbers at tail of arrow indicated percentage of destruction of species by indicated reaction
Numbers at head of arrow indicate percentage of production of species by indicated reaction
(Input and output of reactor not included)
Reactants and products (circled) indicated at arrows.

CH_4
CH_3
CH_3O
CH_2O
CH_2
CHO
CH
CO
CHN
CO_2
CN
N_2
N
NO
NO_2
+H
+OH
+H+M
+O
+M
+O+M
+NO
$+O_2$
+CH4
+CH
$+HO_2$
0.19
0.12
41
56
12
61
76
62
57
15
14
23
21
92
89
11
9
100
96
68
17
20
31
16
24
18
40
81
36
8
63
97
52
33
42
4
83
25
7
5

FIGURE C-2

MAJOR KINETIC PATHS FOR METHANE AIR COMBUSTION COUPLED TO NO_X FORMATION STIRRED REACTOR, 100% STOICHIOMETRIC AIR, τ = 2 msec



LEGEND

Numbers at tail of arrow indicated percentage of destruction of species by indicated reaction

Numbers at head of arrow indicate percentage of production of species by indicated reaction

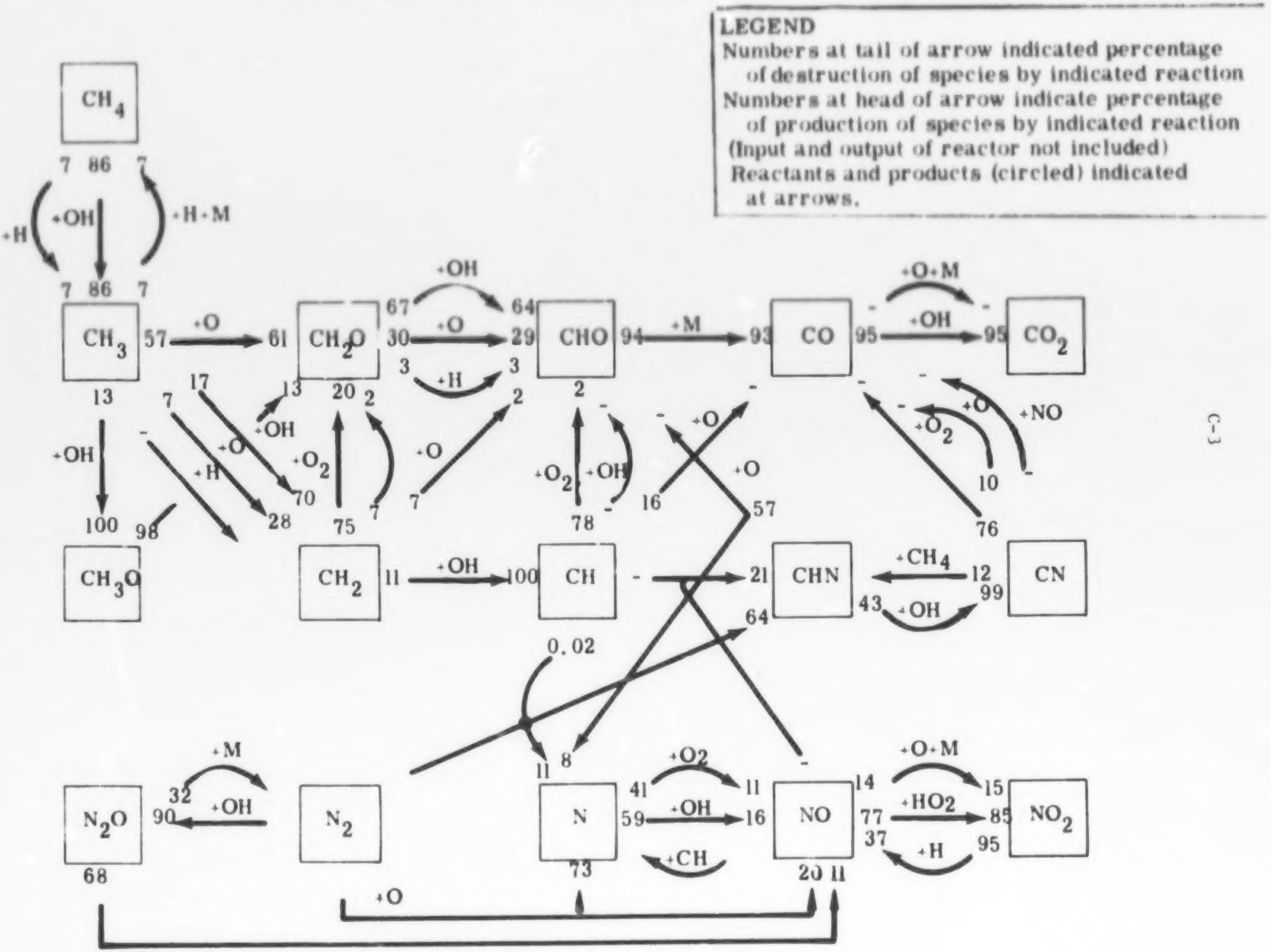
(Input and output of reactor not included)

Reactants and products (circled) indicated at arrows.

CH4
CH3
CH3O
CH2O
CH2
CHO
CH
CO
CO2
CHN
CN
N2
N
NO
NO2
+H
+OH
+H+M
+O
+M
+O+M
+O2
+NO
+CH4
+CH
+HO2
16
79
-
60
67
68
63
25
23
7
6
17
12
14
4
11
100
97
22
70
49
16
12
3
93
91
7
93
55
9
29
81
21
52
99
31
24
19
58
0.08
19
23
17
83
9
40
14
13
51
23
21
98
42
21

FIGURE C-3

MAJOR KINETIC PATHS FOR METHANE AIR COMBUSTION COUPLED TO NO_X FORMATION
STIRRED REACTOR, 125% STOICHIOMETRIC AIR, τ = 2 msec



LEGEND
Numbers at tail of arrow indicated percentage of destruction of species by indicated reaction
Numbers at head of arrow indicate percentage of production of species by indicated reaction
(Input and output of reactor not included)
Reactants and products (circled) indicated at arrows.

CH_4
CH_3
CH_2O
CHO
CO
CO_2
CH_3O
CH_2
CH
CHN
CN
N_2O
N_2
N
NO
NO_2
+H
+OH
+H+M
+O
+O_2
+M
+O+M
+NO
+CH_4
+CH
+O2
+HO2
7
86
57
61
67
30
3
64
29
94
93
95
13
17
20
2
100
98
28
70
75
78
16
10
76
11
21
12
99
43
0.02
57
64
8
32
90
41
59
14
77
37
15
85
68
73
20